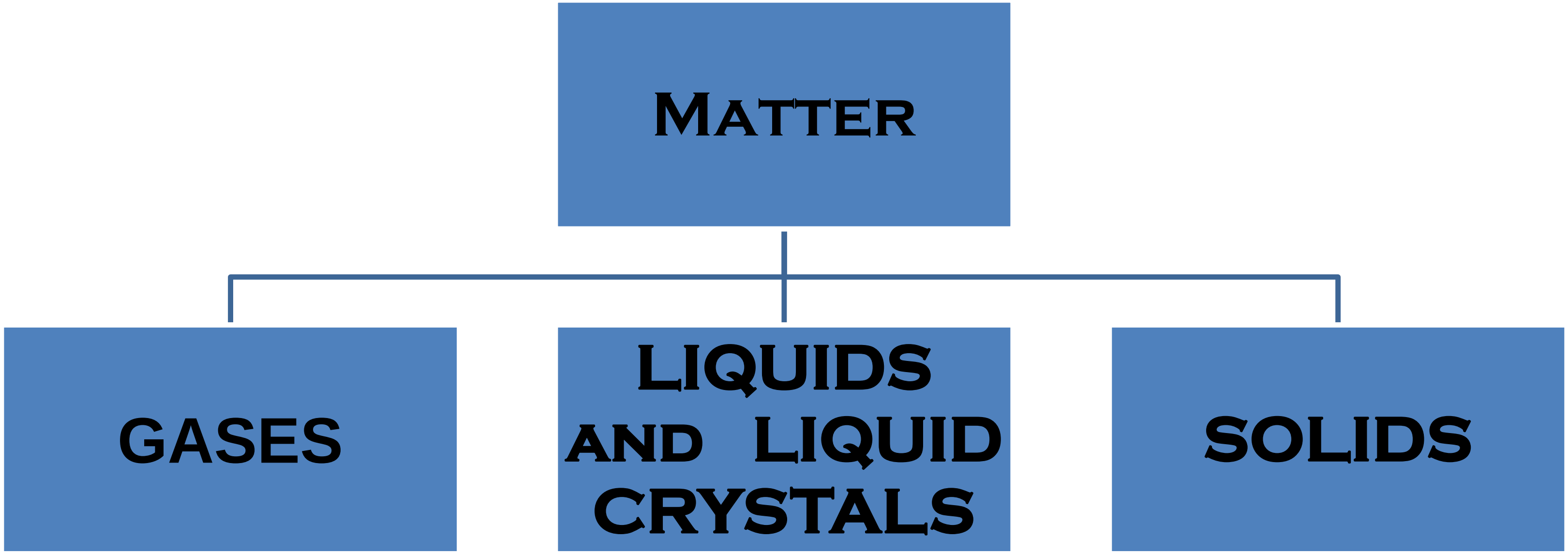

यदि परिस्थितियों पर आपकी मजबूत
पकड़ है तो जहर उगलने वाले भी
आपका कुछ नहीं बिगाड़ सकते हैं

CHAPTER 1.
CRYSTAL STRUCTURE

- Elementary Crystallography
  - Solid materials (crystalline, polycrystalline, amorphous)
  - Crystallography
  - Crystal Lattice
  - Crystal Structure
  - Types of Lattices
  - Unit Cell
  - Directions-Planes-Miller Indices in Cubic Unit Cell
- Typical Crystal Structures (3D– 14 Bravais Lattices and the Seven Crystal System)
- Elements of Symmetry

MATTER



MATTER

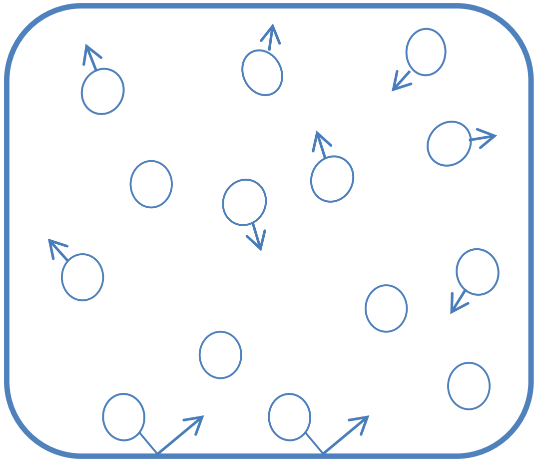
GASES

LIQUIDS AND LIQUID CRYSTALS

SOLIDS

Gases

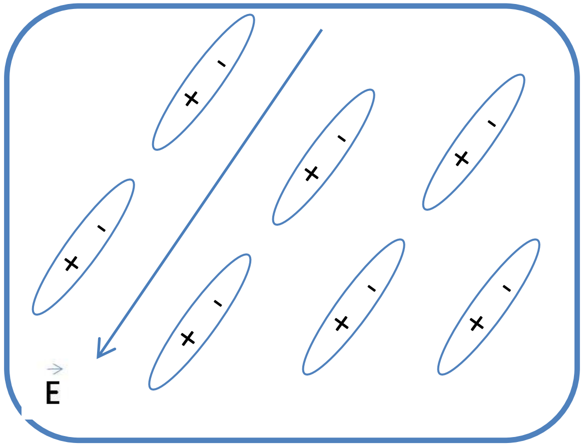
- Gases have atoms or molecules that do not bond to one another in a range of pressure, temperature and volume.
- These molecules haven't any particular order and move freely within a container.



Liquids and Liquid Crystals

- Similar to gases, liquids haven’t any atomic/molecular order and they assume the shape of the containers.
- Applying low levels of thermal energy can easily break the existing weak bonds.

Liquid crystals have mobile molecules, but a type of long range order can exist; the molecules have a permanent dipole. Applying an electric field rotates the dipole and establishes order within the collection of molecules.

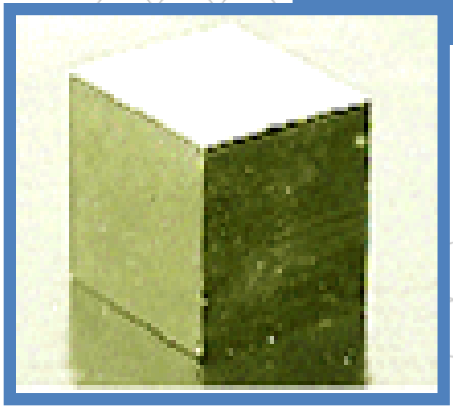


Solids

- Solids consist of atoms or molecules ***executing thermal motion*** about an equilibrium position ***fixed at a point*** in space.
- Solids can take the form of crystalline, polycrstalline, or amorphous materials.
- Solids (at a given temperature, pressure, and volume) have stronger bonds between molecules and atoms than liquids.
- Solids require more energy to ***break the bonds.***

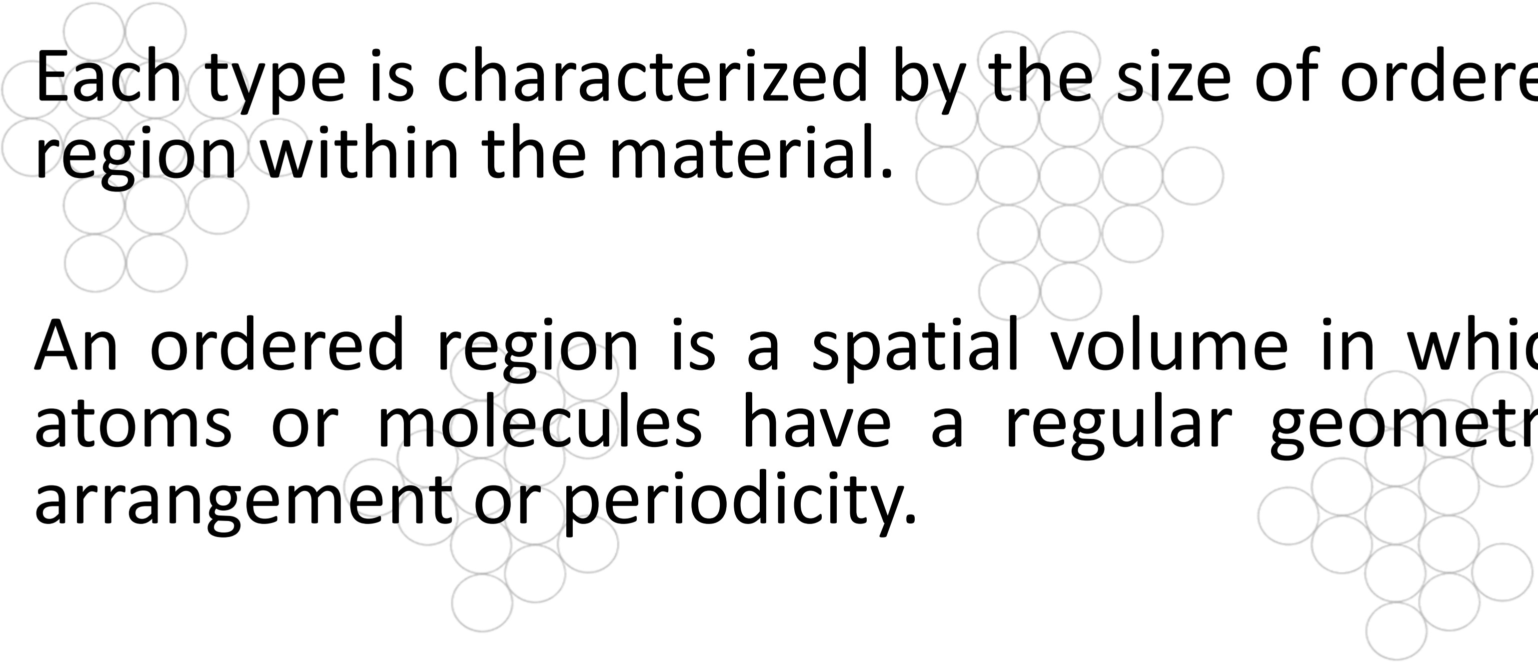
SOLID MATERIALS

- **CRYSTALLINE**
  - **Single Crystal**
- **POLYCRYSTALLINE**
- **AMORPHOUS (Non-crystalline)**



Types of Solids

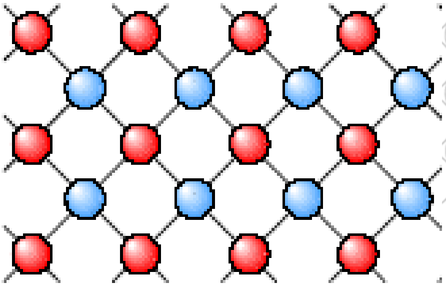
- Single crystal, polycrystalline, and amorphous, are the three general types of solids.

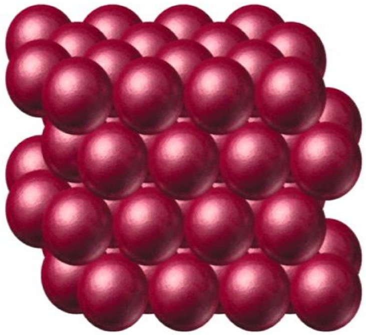


- Each type is characterized by the size of ordered region within the material.
- An ordered region is a spatial volume in which atoms or molecules have a regular geometric arrangement or periodicity.

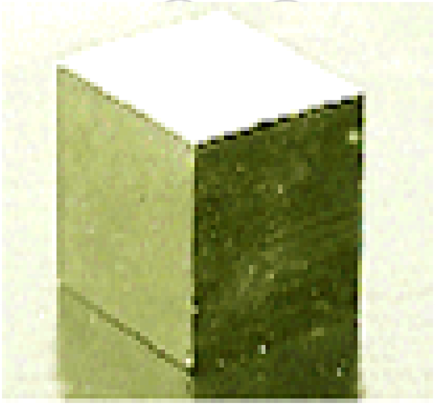
Crystalline Solid

- Crystalline Solid is the solid form of a substance in which the ***atoms or molecules*** are arranged in a definite, repeating pattern in three dimension.
- Single crystals, ideally have a high degree of order, or regular geometric periodicity, throughout the ***entire volume of the material***.



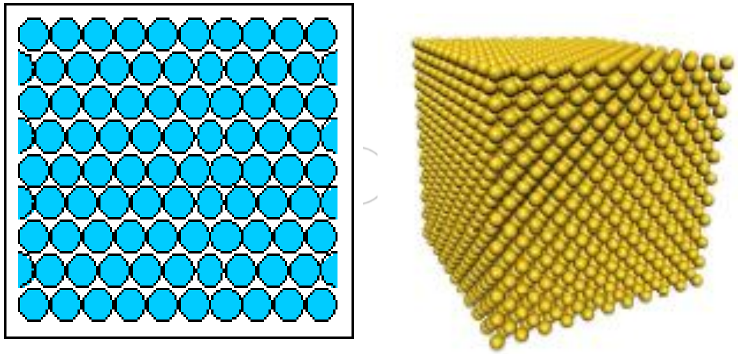


(a) Crystalline solid

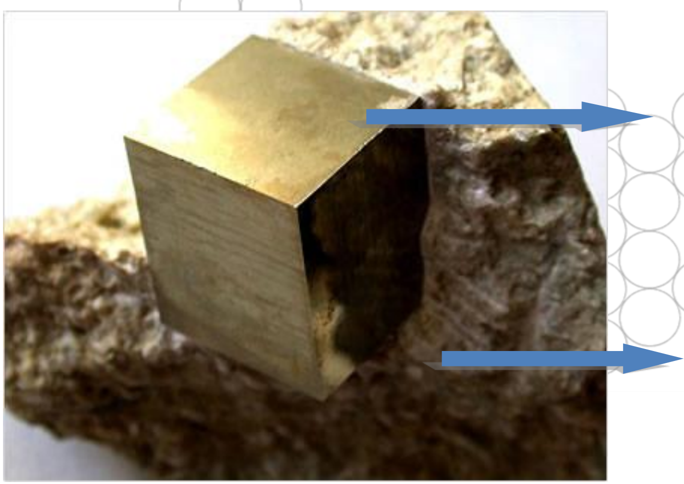


Crystalline Solid

- Single crystal has an atomic structure that repeats periodically across its whole volume. Even at infinite length scales, each atom is related to every other equivalent atom in the structure by translational symmetry



Single Crystal

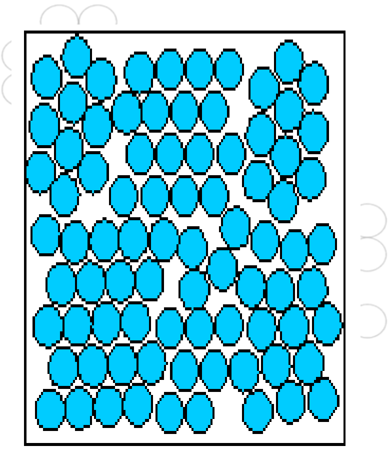


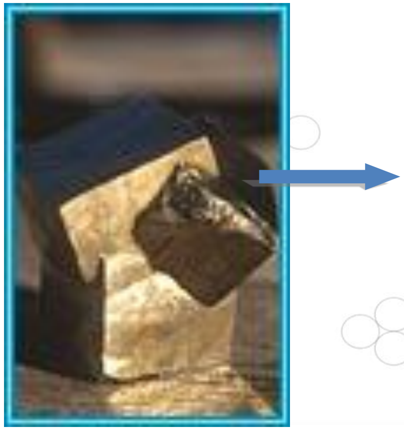
Single Pyrite Crystal

Amorphous Solid

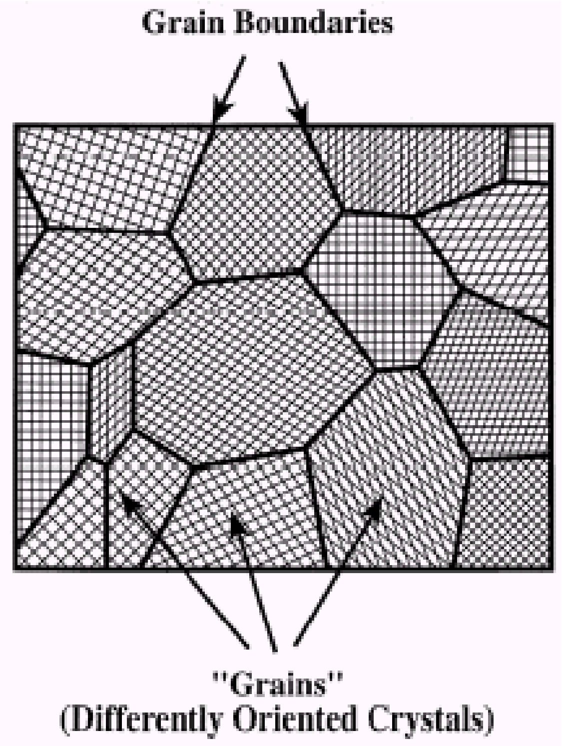
Polycrystalline Solid

- Polycrystal is a material made up of an aggregate of *many small single crystals* (also called crystallites or grains).
- Polycrystalline material have a high degree of order over many atomic or molecular dimensions.





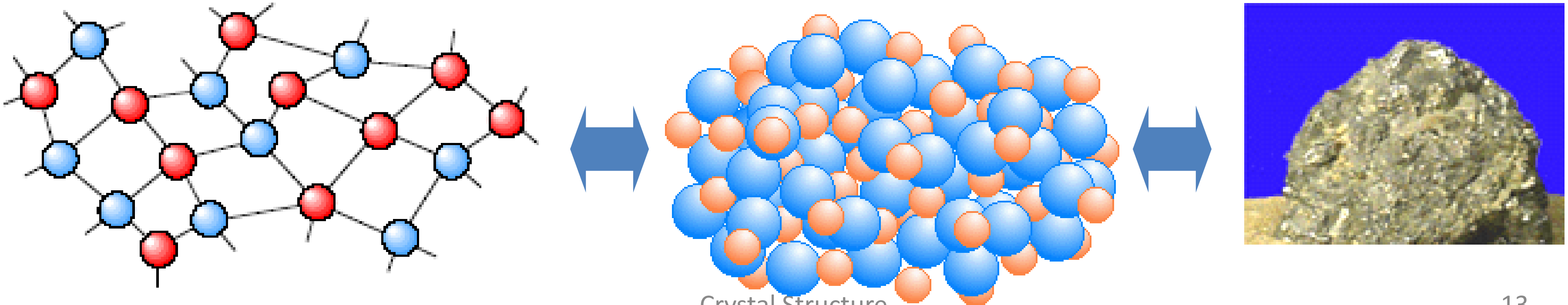
Polycrystalline
Pyrite form
(Grain)



- These *ordered regions,* or single crytal regions, vary in size and orientation wrt one another.
- These regions are called as *grains (domain)* and are separated from one another by *grain boundaries. The atomic order can vary from one domain to the next.*
- The grains are usually *100 nm - 100 microns in diameter*.
- Polycrystals with grains that are <10 nm in diameter are called nanocrystalline

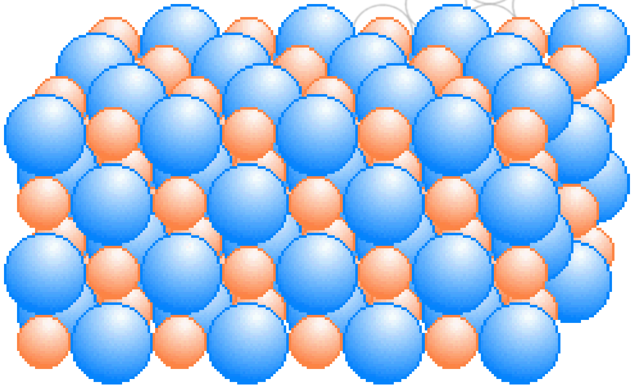
Amorphous Solid

- Amorphous (Non-crystalline) Solid is composed of randomly orientated atoms , ions, or molecules that do not form defined patterns or lattice structures.
- Amorphous materials have order only within a few atomic or molecular dimensions.
- Amorphous solid have no sharp melting point.
- Amorphous materials do not have any long-range order, but they have varying degrees of short-range order.
- Examples to amorphous materials include amorphous silicon, plastics, and glasses.
- Amorphous silicon can be used in solar cells and thin film transistors.



Departure From Perfect Crystal

- Strictly speaking, one cannot prepare a perfect crystal. For example, even the surface of a crystal is a kind of imperfection because the periodicity is interrupted there.
- Another example concerns the thermal vibrations of the atoms around their equilibrium positions for any temperature T>0°K.

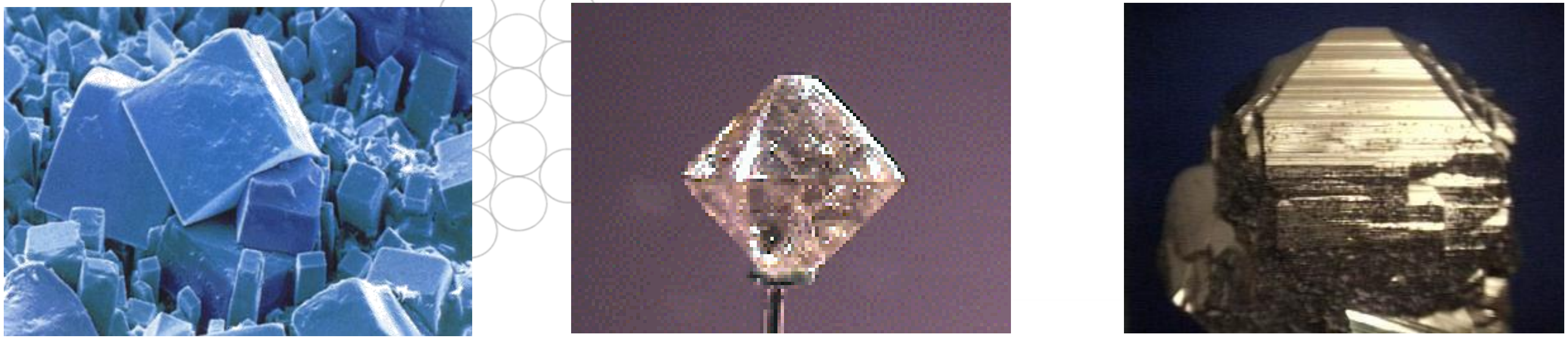


- As a third example, actual crystal always contains some foreign atoms, i.e., impurities. These impurities spoils the perfect crystal structure.

CRYSTALLOGRAPHY

What is crystallography?

The branch of science that deals with the geometric description of crystals and their internal arrangement.

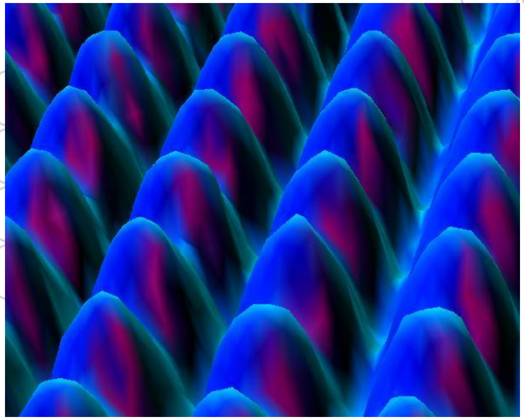


CRYSTAL LATTICE

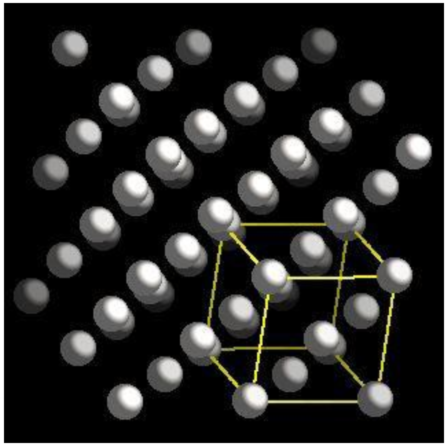
What is crystal (space) lattice?

In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.

Platinum



Platinum surface
(scanning tunneling microscope)



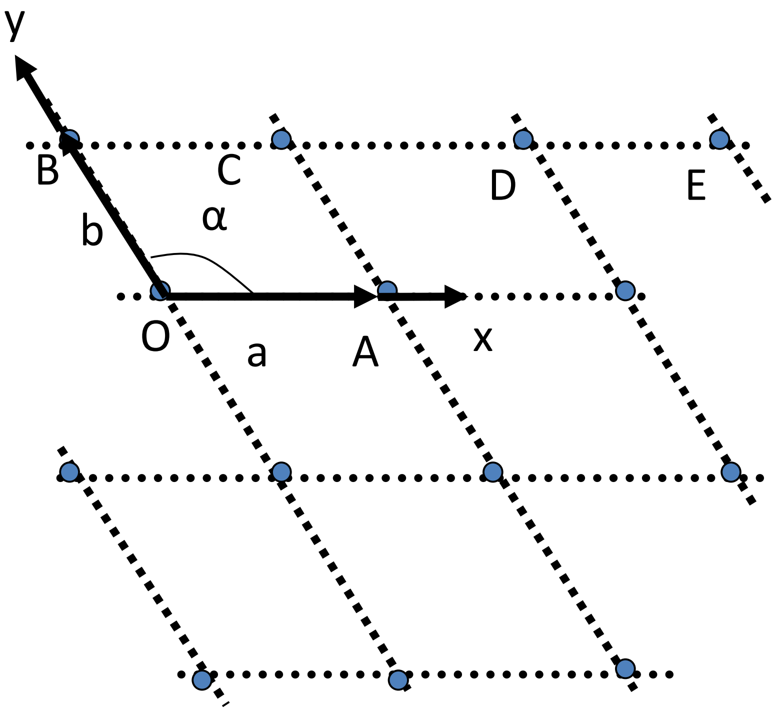
Crystal lattice and
structure of Platinum

ELEMENTARY CRYSTALLOGRAPHY

- A basic knowledge of crystallography is essential for solid state physicists;
  - to specify any crystal structure and
  - to classify the solids into different types according to the symmetries they possess.
- Symmetry of a crystal can have a profound influence on its properties.
- We will concern in this course with solids with simple structures.

Crystal Lattice

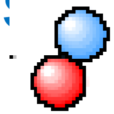
- An infinite array of points in space,
- Each point has identical surroundings to all others.
- Arrays are arranged exactly in a periodic manner.

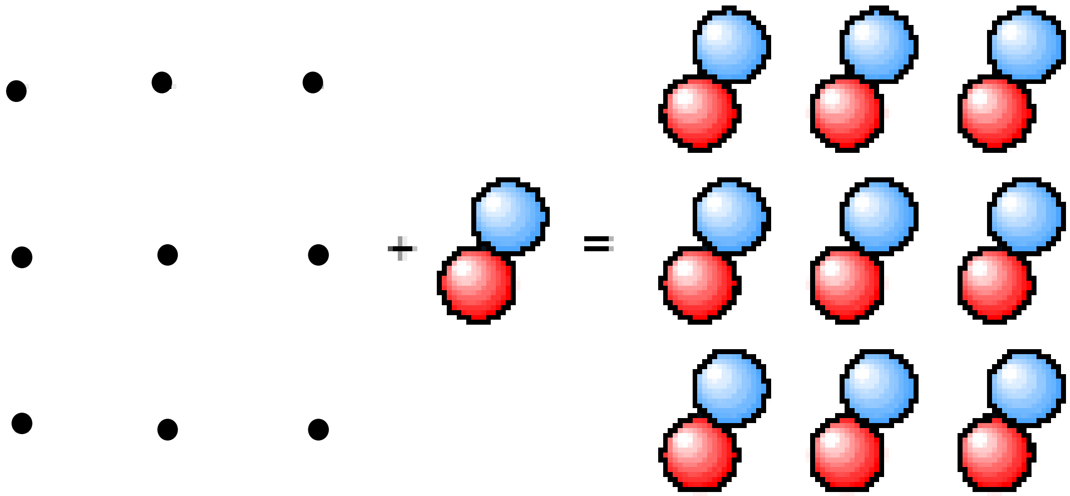


Crystal Structure

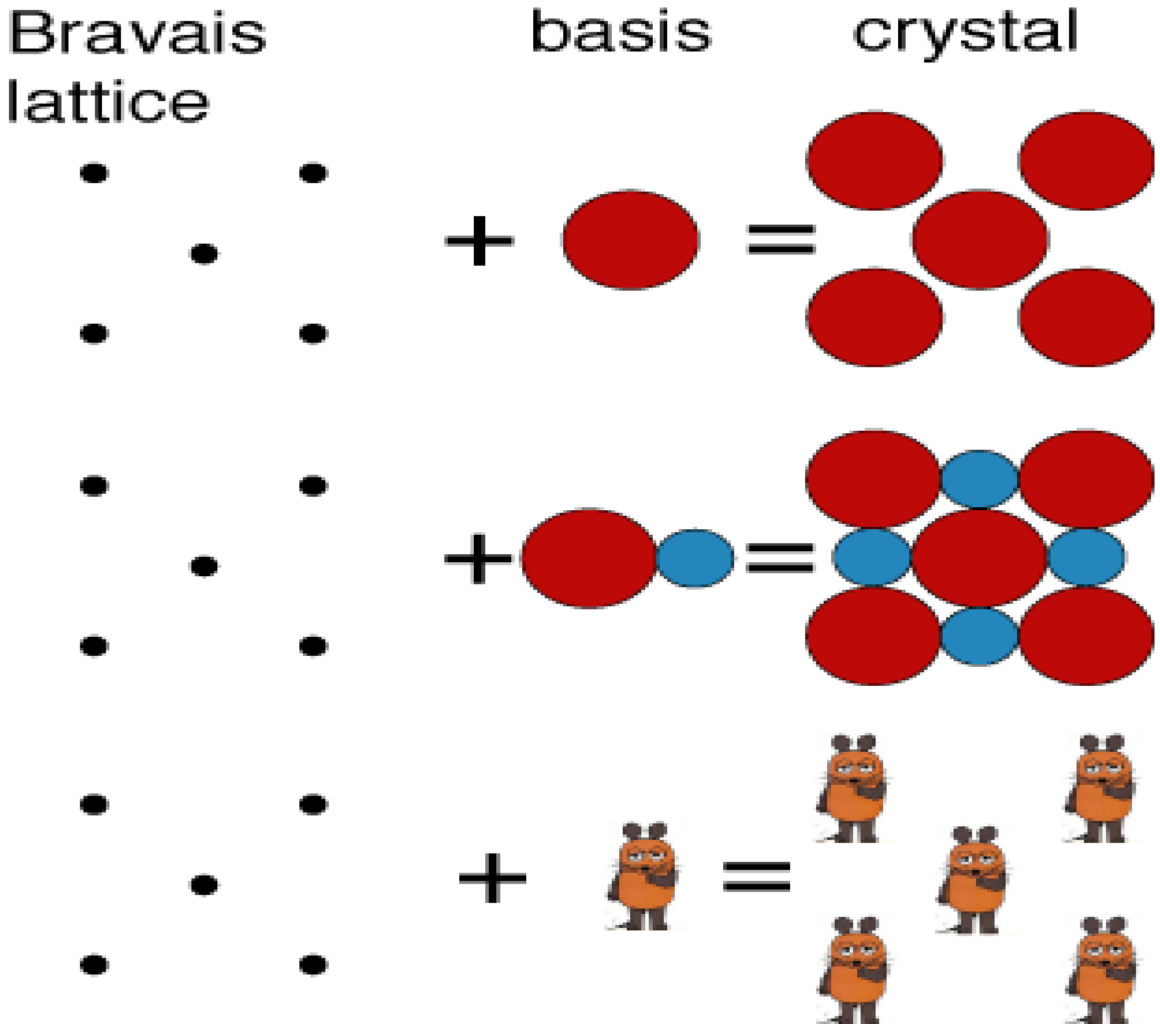
- Crystal structure can be obtained by attaching atoms, groups of atoms or molecules which are called basis (motif) to the lattice sides of the lattice point.

Crystal Structure = Crystal Lattice ● + Basis



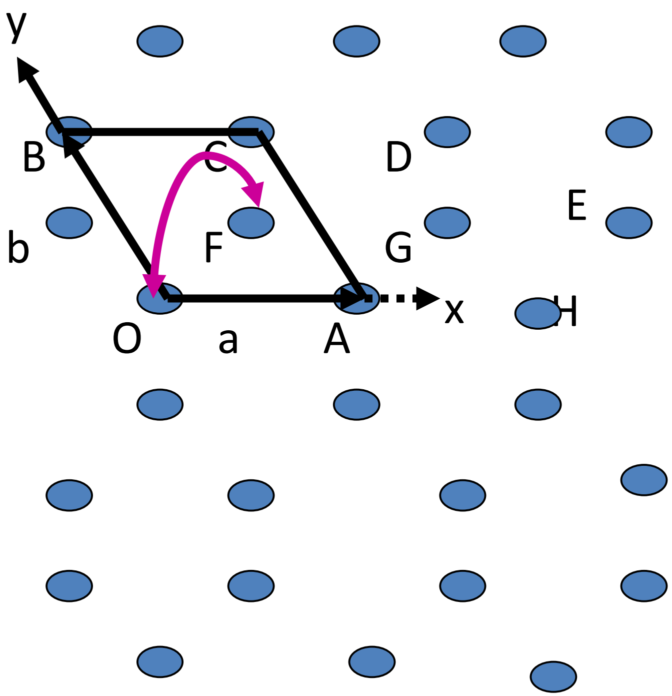


A two-dimensional Bravais lattice with different choices for the basis

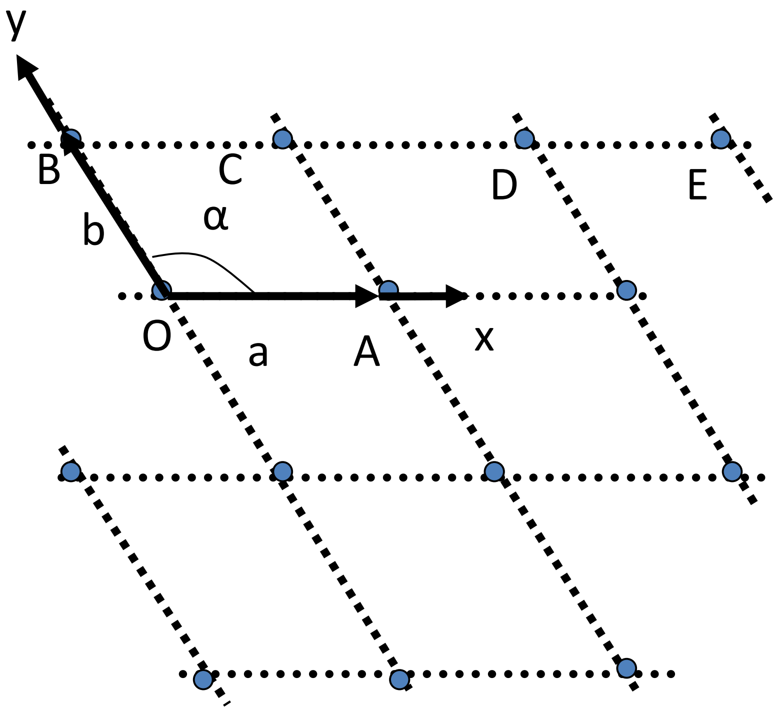


Basis [Motif]

- A group of atoms which describe crystal structure



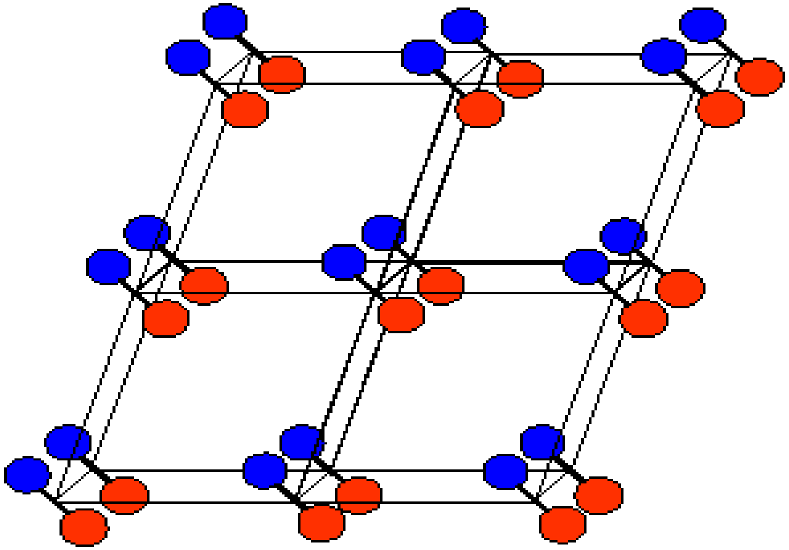
a) Situation of atoms at the corners of regular hexagons

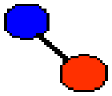


b) Crystal lattice obtained by identifying all the atoms in (a)

Crystal structure

- Don't mix up atoms with lattice points
- Lattice points are infinitesimal points in space
- Lattice points do not necessarily lie at the centre of atoms



Crystal = Crystal Lattice ● + Basis 
Structure

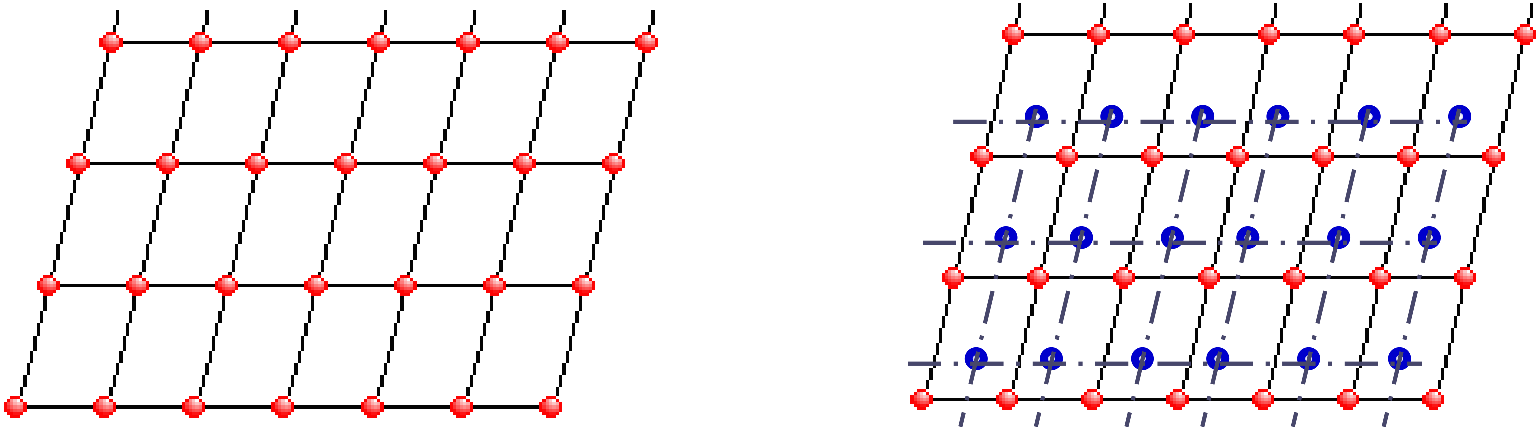
Crystal Lattice

Bravais Lattice (BL)

All atoms are of the same kind
All lattice points are equivalent

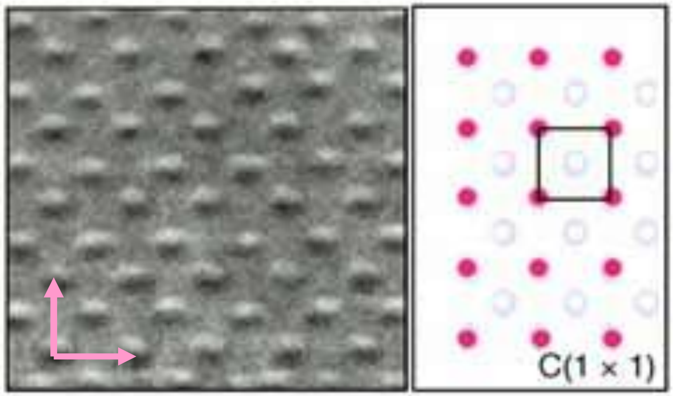
Non-Bravais Lattice (non-BL)

Atoms can be of different kind
Some lattice points are not equivalent
A combination of two or more BL



Types Of Crystal Lattices

1) Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed. Lattice is invariant under a translation.



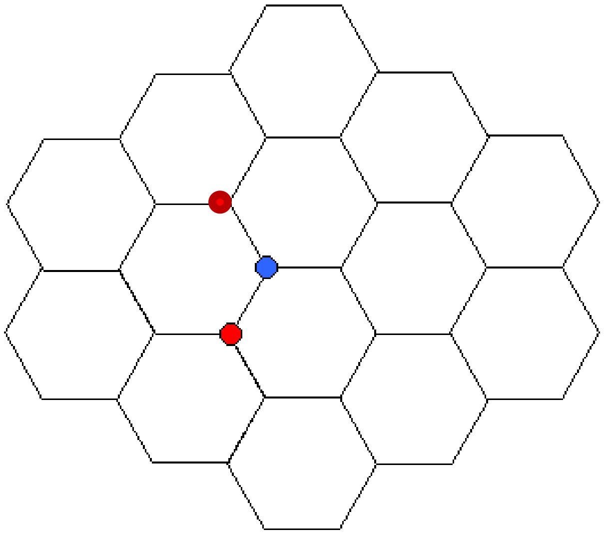
Nb film

Types Of Crystal Lattices

2) Non-Bravais Lattice

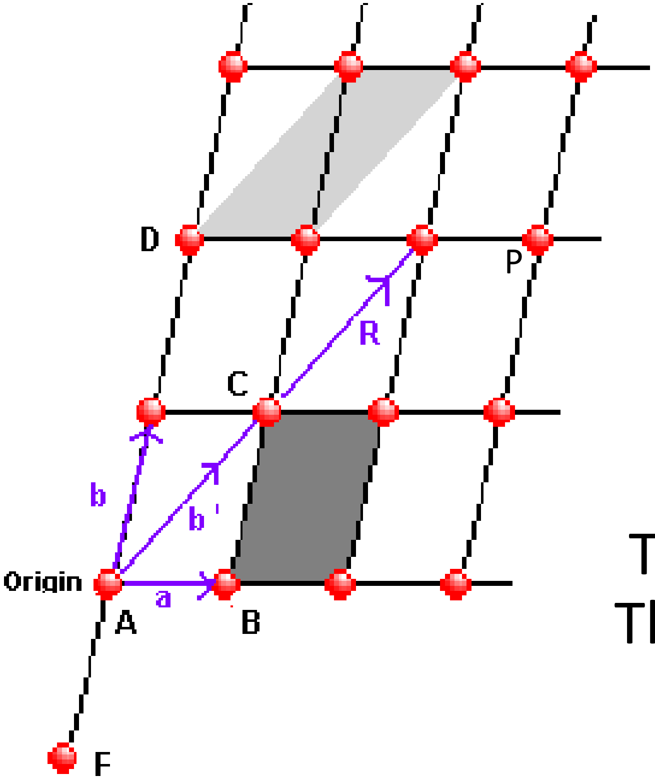
Not only the arrangement but also the orientation must appear exactly the same from every point in a bravais lattice.

- The red side has a neighbour to its immediate left, the blue one instead has a neighbour to its right.
- Red (and blue) sides are equivalent and have the same appearance
- Red and blue sides are not equivalent. Same appearance can be obtained rotating blue side 180º.



Honeycomb

Translational Lattice Vectors – 2D



Point D(n1, n2) = (0,2)

Point F (n1, n2) = (0,-1)

A space lattice is a set of points such that a translation from any point in the lattice by a vector;

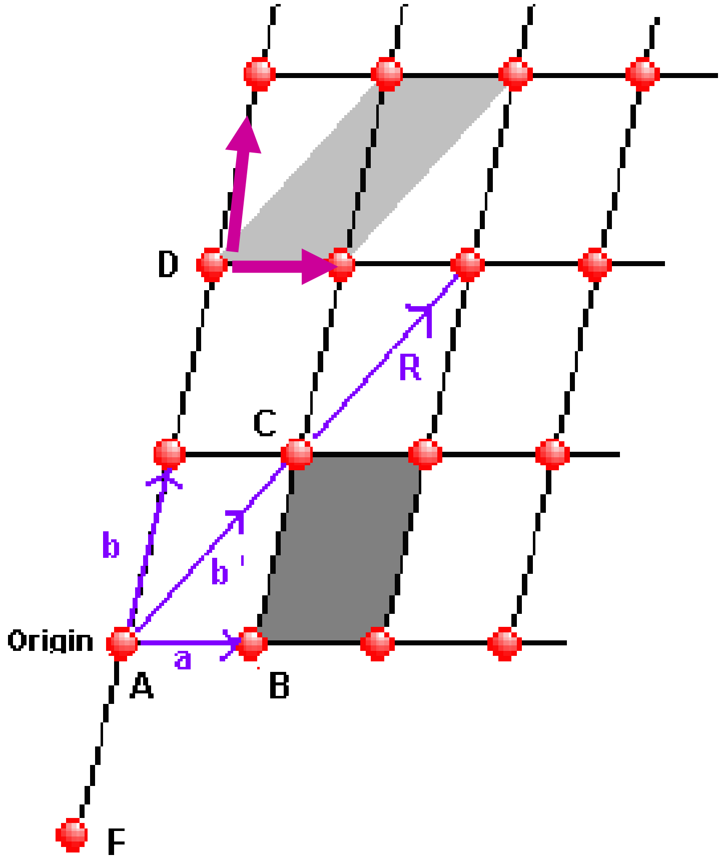
$$R_n = n_1 a + n_2 b$$

locates an exactly *equivalent* point, *i.e.* a point with the same environment as *P* .

This is translational symmetry.

The vectors *a, b* are known as lattice vectors and (n_1, n_2) is a pair of integers whose values depend on the lattice point.

Lattice Vectors – 2D

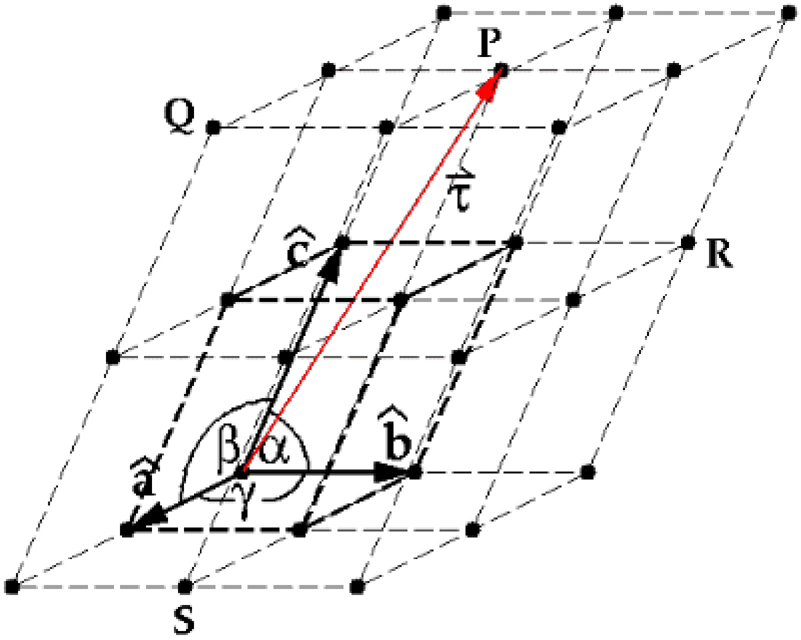


- The <u>two vectors a</u> and <u>b</u> form a set of lattice vectors for the lattice.

- ***The choice of lattice vectors is not unique***. Thus one could equally well take the <u>vectors a and b' as a lattice vectors.</u>

Lattice Vectors – 3D

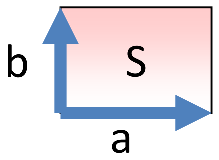
An ideal three dimensional crystal is described by 3 fundamental translation vectors a, b and c. If there is a lattice point represented by the position vector R, there is then also a lattice point represented by the position vector where *u*, *v* and *w* are arbitrary integers.



$$R = u\,a + v\,b + w\,c$$

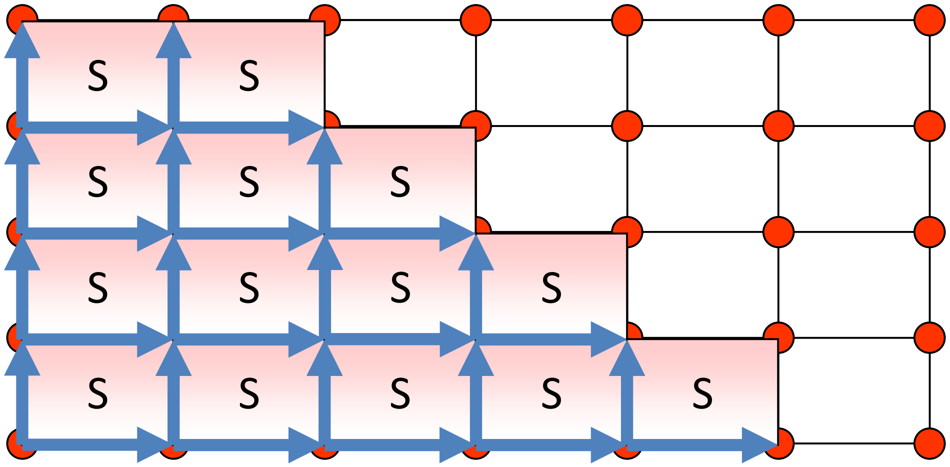
Unit Cell in 2D

- The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.



Unit Cell

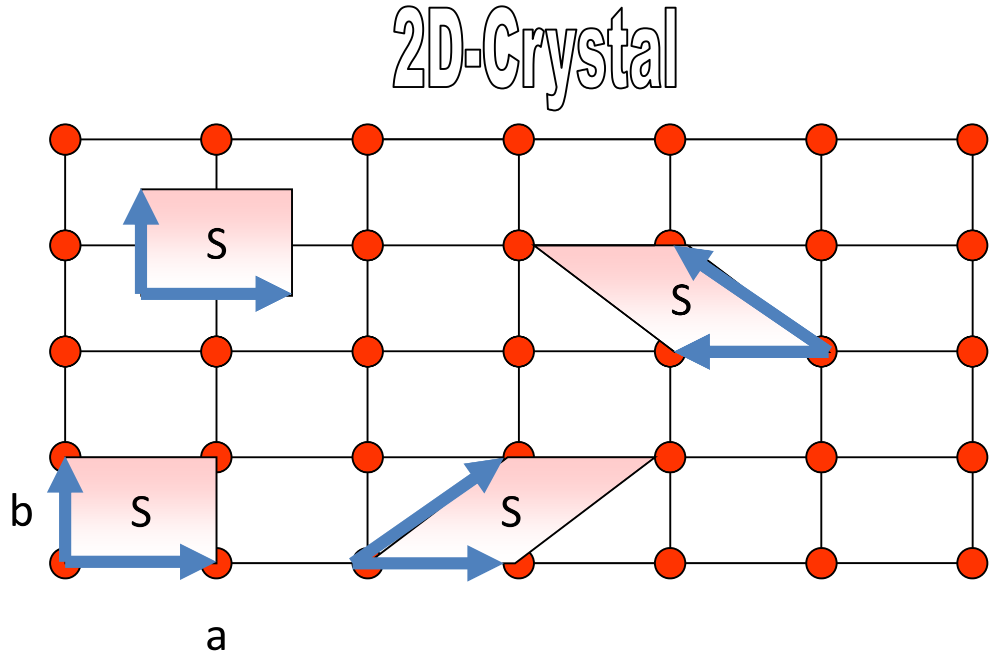
2D-Crystal



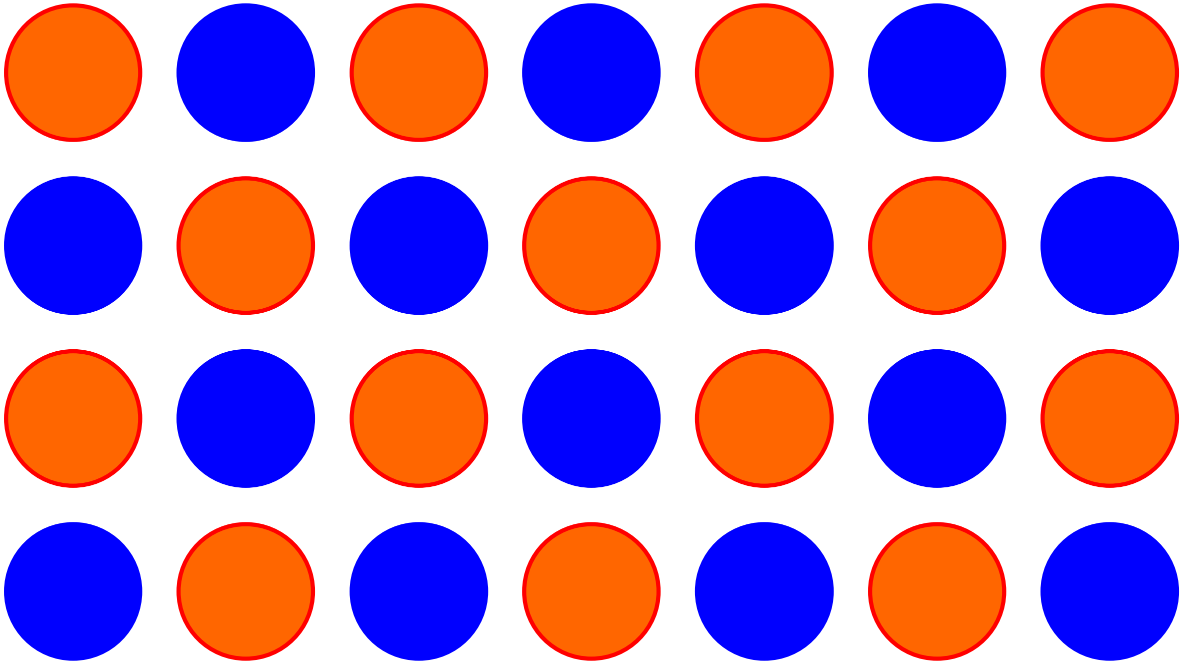
Unit Cell in 2D

- The smallest component of the crystal (group of atoms, ions or molecules), which <u>when stacked together</u> with pure translational repetition reproduces the whole crystal.

The choice of unit cell is not unique.

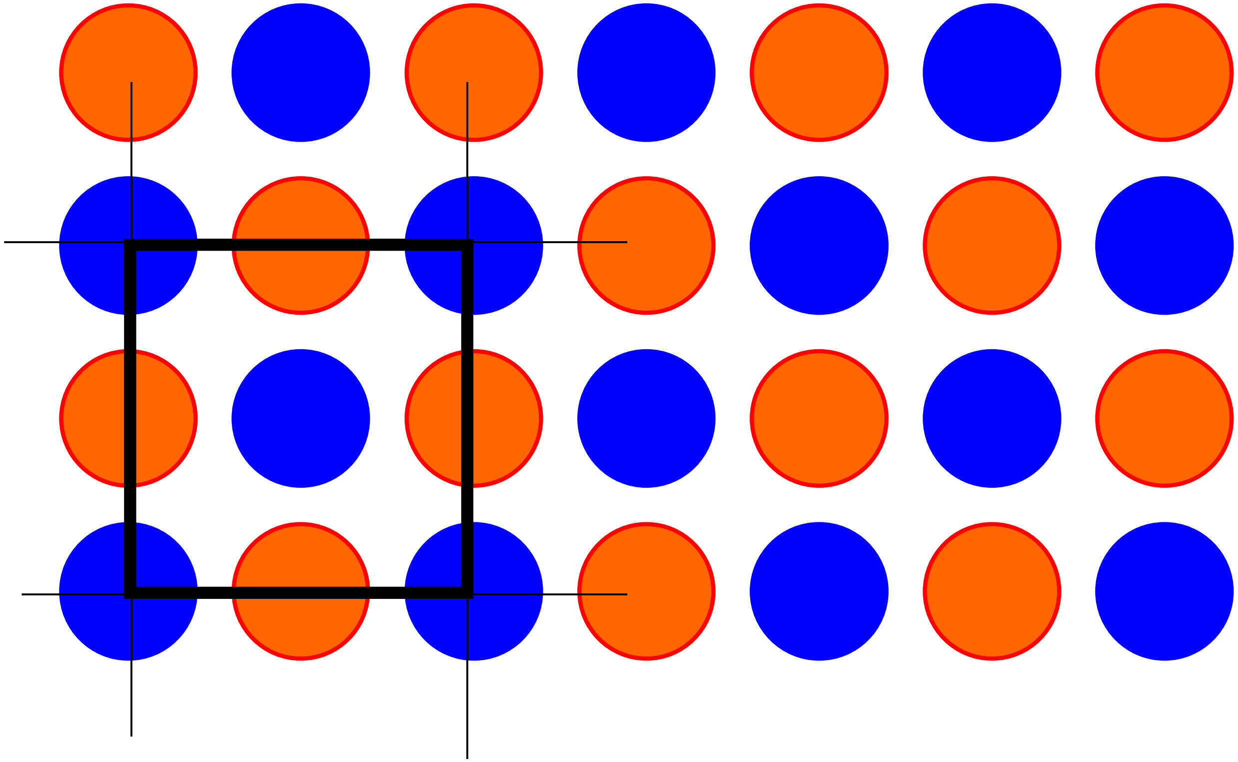


2D Unit Cell example -(NaCl)

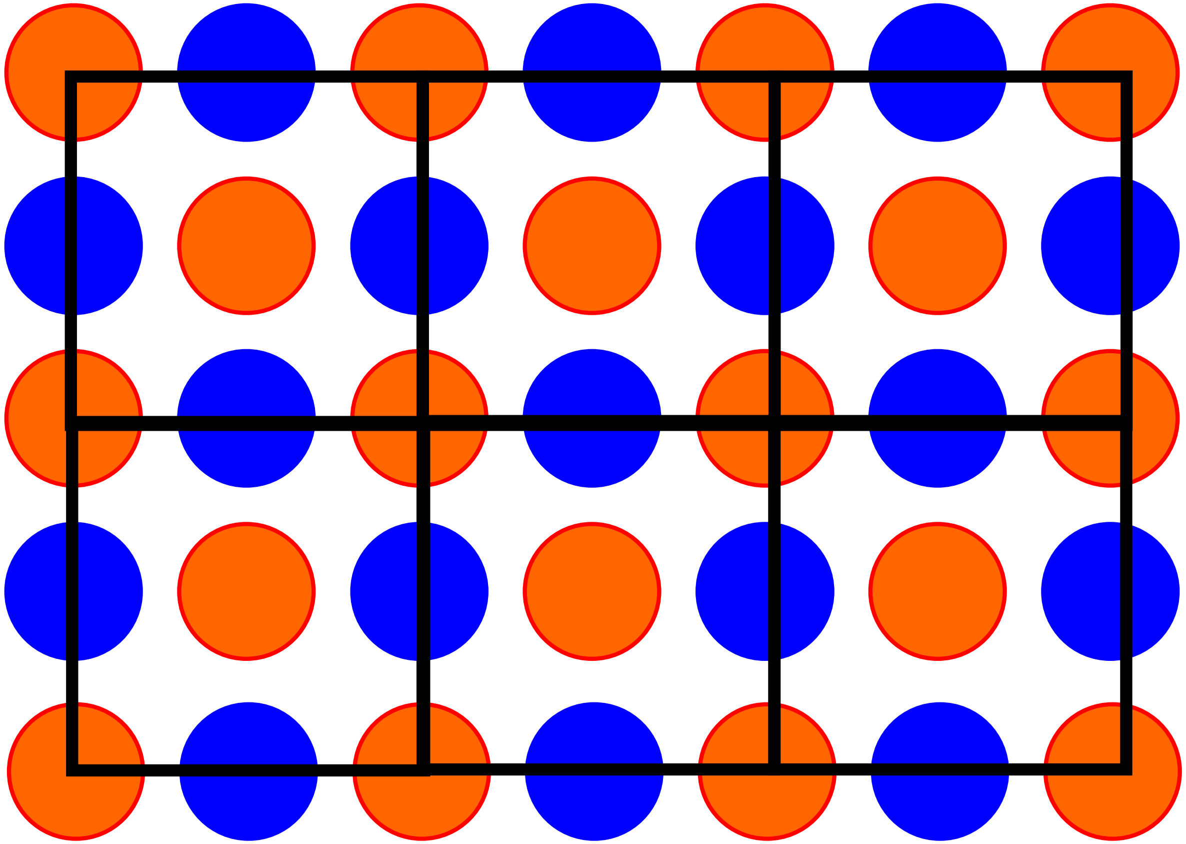


We define <u>lattice points</u> ; these are points with *identical environments*

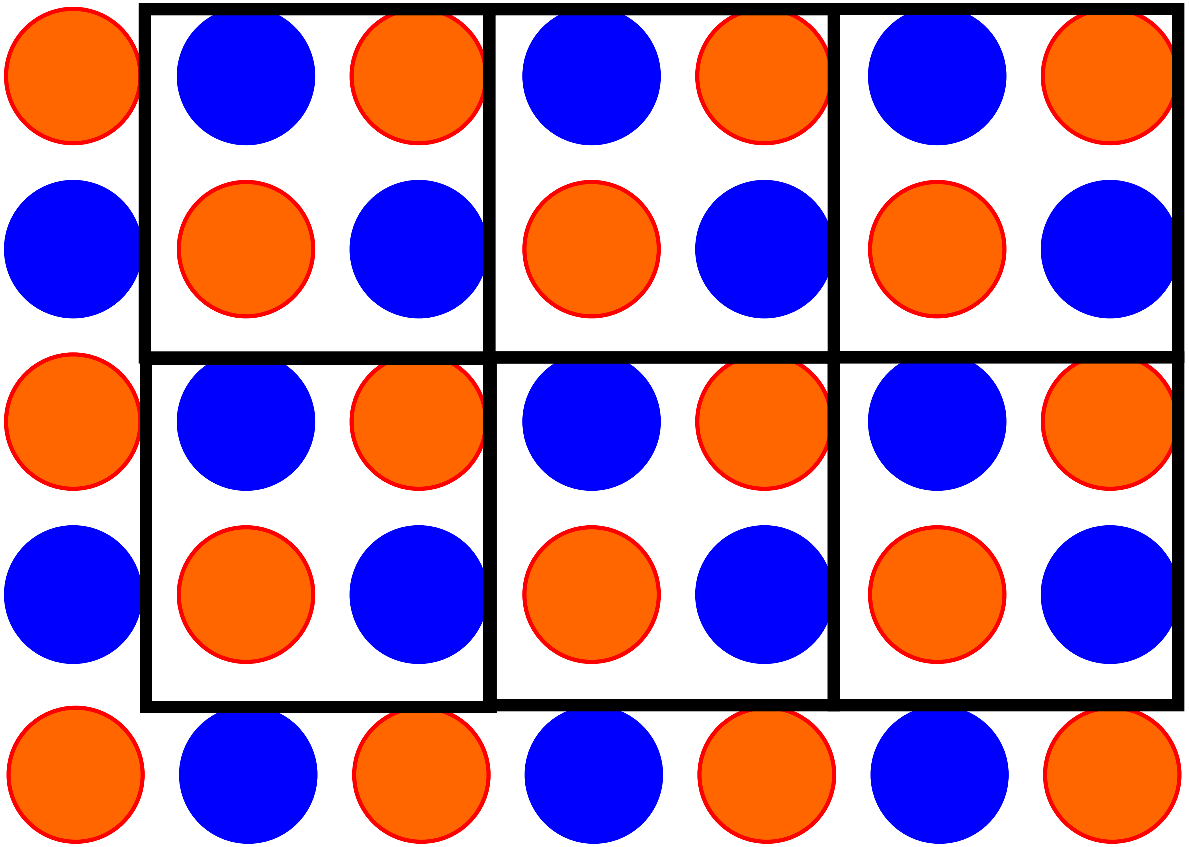
Choice of origin is arbitrary - lattice points need not be atoms - **but** unit cell size should always be the same.



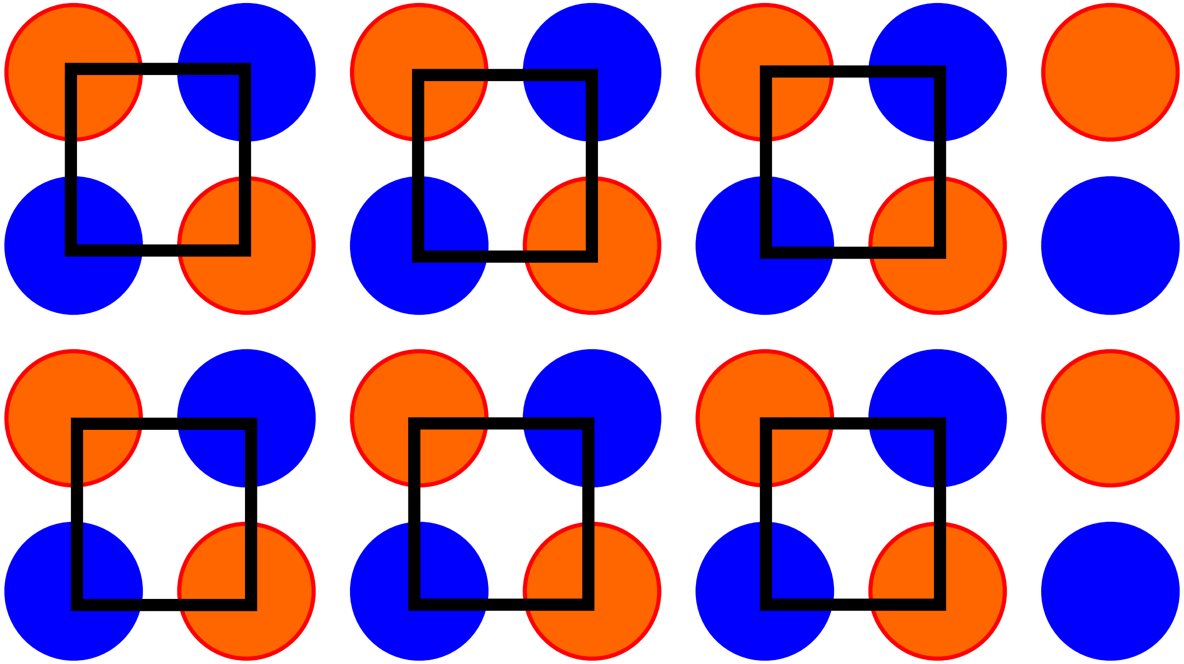
This is also a unit cell -
it doesn’t matter if you start from Na or Cl



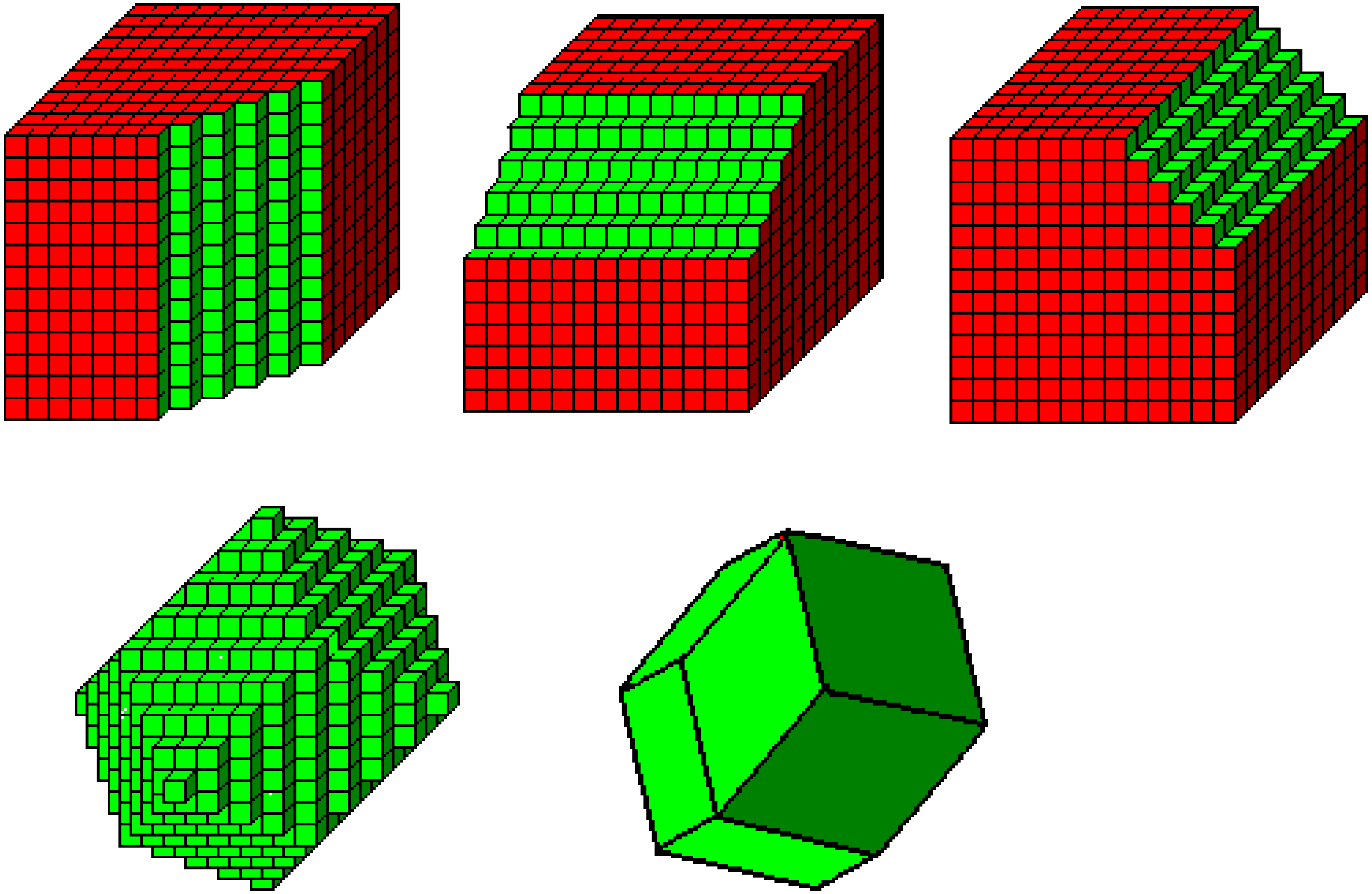
- or if you don’t start from an atom



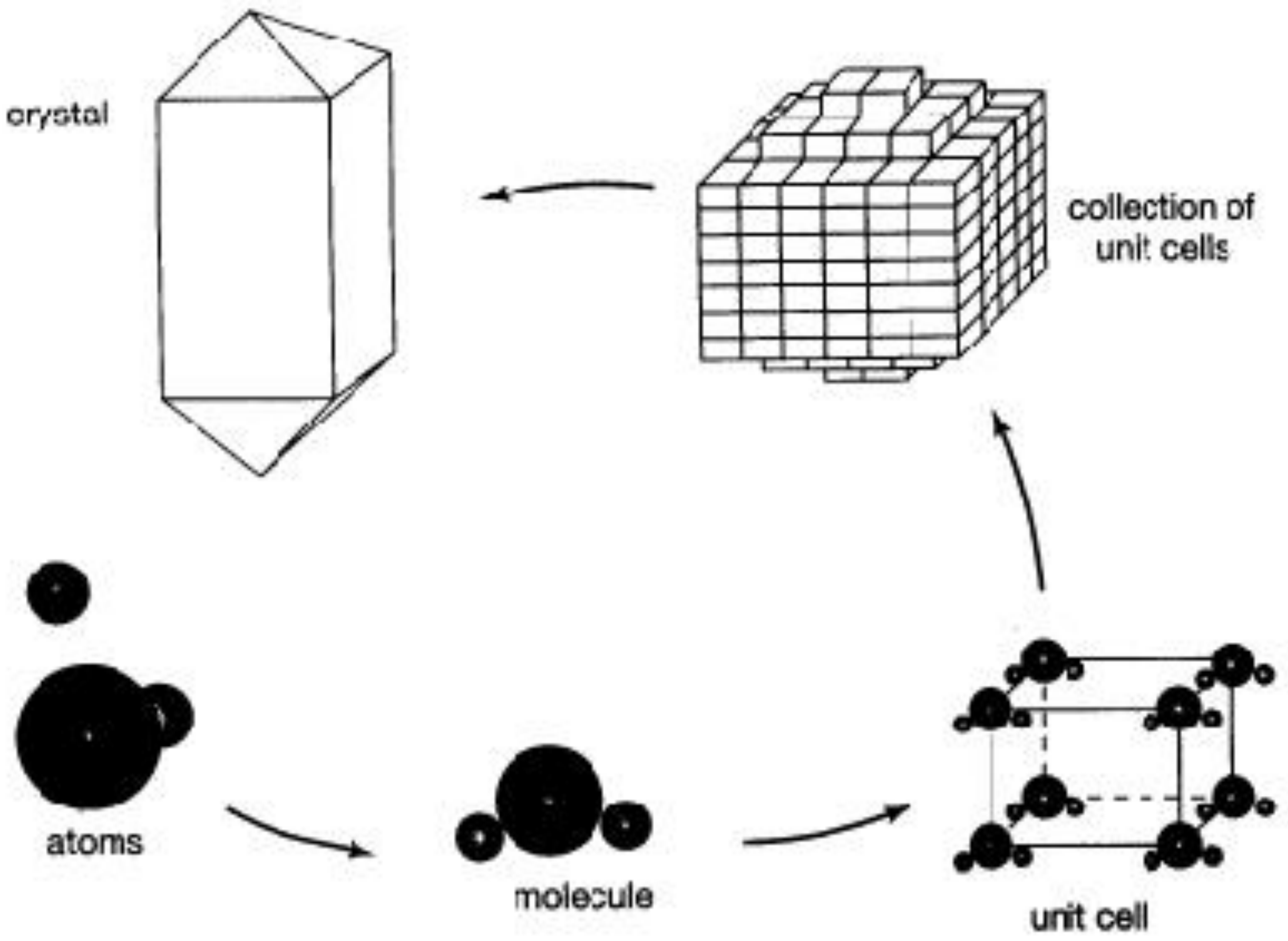
This is NOT a unit cell even though they are all the same - empty space is not allowed!



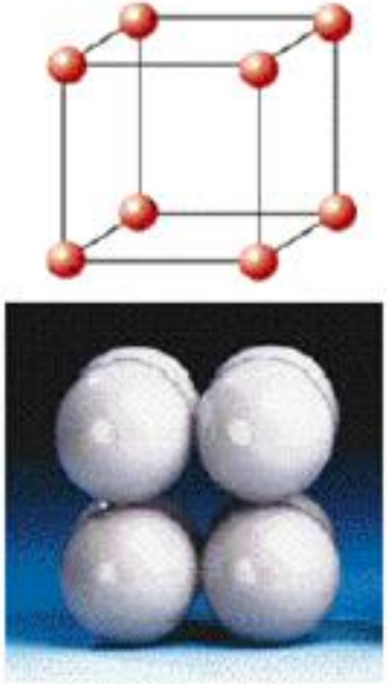
Unit Cell in 3D



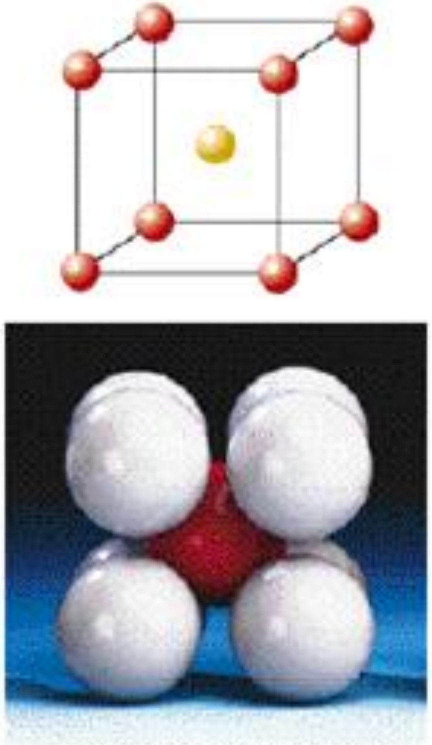
Unit Cell in 3D



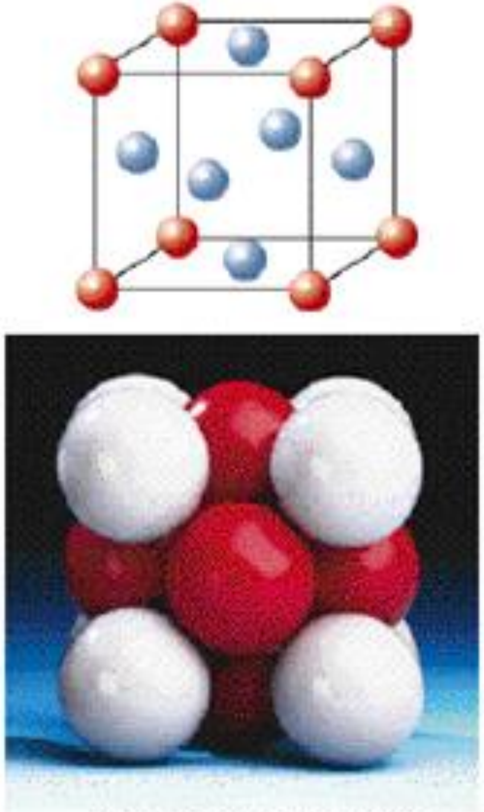
Three common Unit Cell in 3D



simple cubic

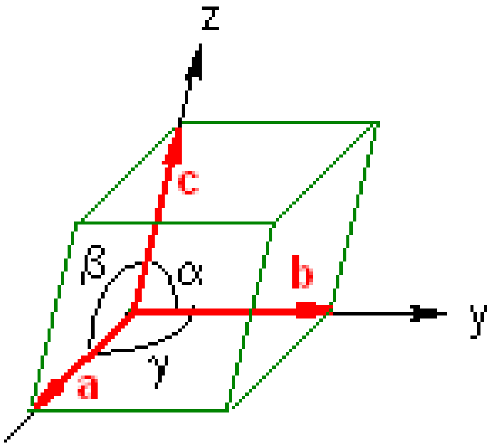


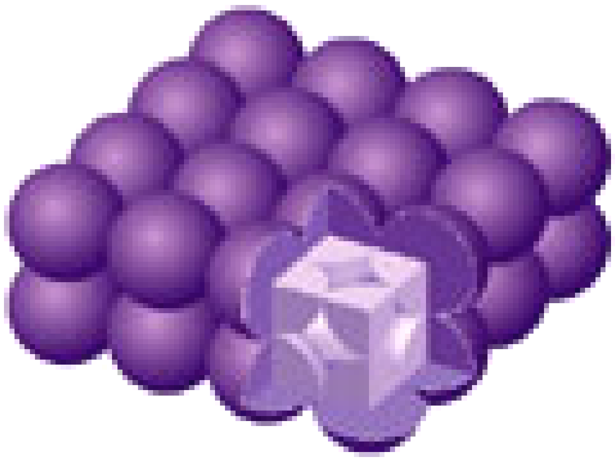
body-centered cubic



face-centered cubic

Unit Cell





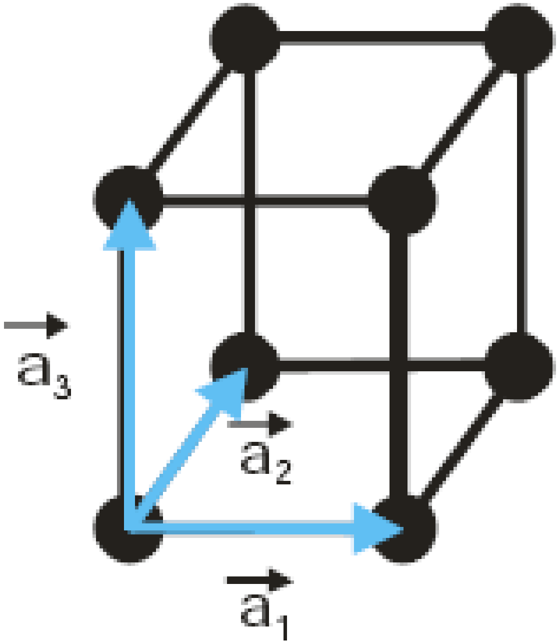
- The unit cell and, consequently, the entire lattice, is *uniquely* determined by the six lattice constants: a, b, c, α, β and γ.
- Only 1/8 of each lattice point in a unit cell can actually be assigned to that cell.
- Each unit cell in the figure can be associated with 8 x 1/8 = 1 lattice point.

Primitive Unit Cell and vectors

- A primitive unit cell is made of primitive translation vectors a_1 ,a_2, and a_3 such that there is no cell of smaller volume that can be used as a building block for crystal structures.

- A primitive unit cell will fill space by repetition of suitable crystal translation vectors. This defined by the parallelpiped a_1, a_2 and a_3. The volume of a primitive unit cell can be found by

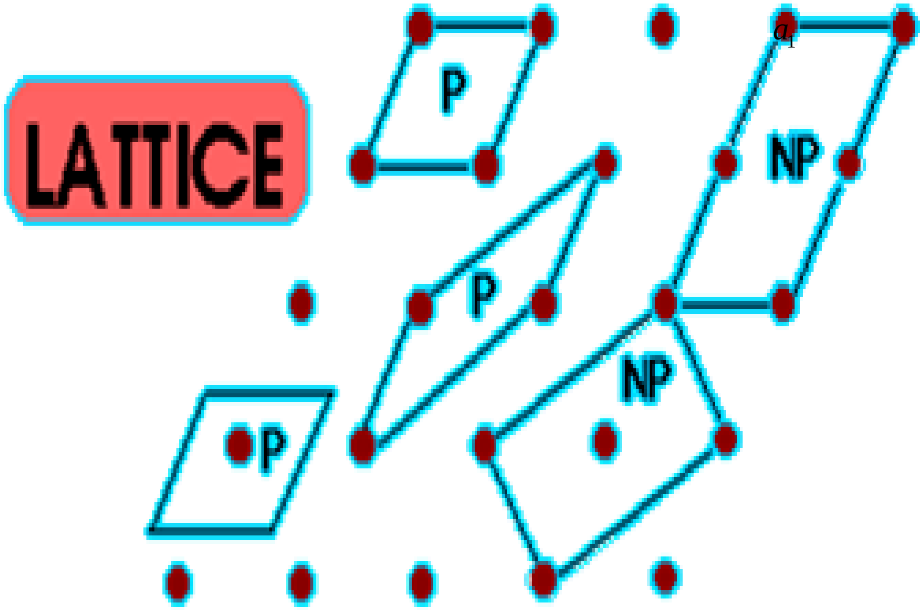
- $V = a_1.(a_2 \times a_3)$ (vector products)



Cubic cell volume = a^3

Primitive Unit Cell

- The primitive unit cell must have only one lattice point.
- There can be different choices for lattice vectors , but the volumes of these primitive cells are all the same.



P = Primitive Unit Cell
NP = Non-Primitive Unit Cell

TYPICAL CRYSTAL STRUCTURES

3D – 14 BRAVAIS LATTICES AND THE SEVEN CRYSTAL SYSTEM

- There are only seven different shapes of unit cell which can be stacked together to completely fill all space (in 3 dimensions) without overlapping.
- This gives the seven crystal systems, in which all crystal structures can be classified.

3D – 14 BRAVAIS LATTICES AND THE SEVEN CRYSTAL SYSTEM

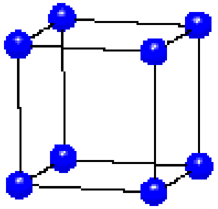
- Cubic Crystal System (SC, BCC,FCC)
- Hexagonal Crystal System (S)
- Triclinic Crystal System (S)
- Monoclinic Crystal System (S, Base-C)
- Orthorhombic Crystal System (S, Base-C, BC, FC)
- Tetragonal Crystal System (S, BC)
- Trigonal (Rhombohedral) Crystal System (S)

CUBIC

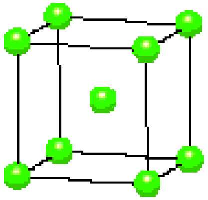
$a = b = c$

$\alpha = \beta = \gamma = 90°$

P



I



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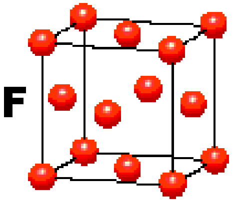
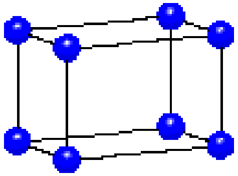


TETRAGONAL

$a = b \neq c$

$\alpha = \beta = \gamma = 90°$

P



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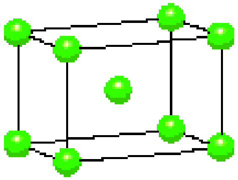
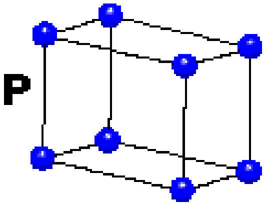


ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

P



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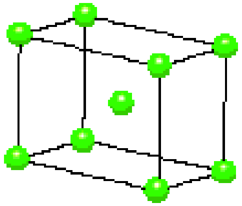

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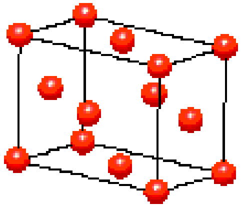
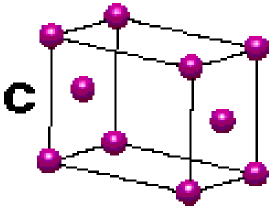


C



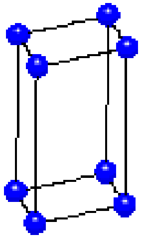
HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

$\gamma = 120°$

P

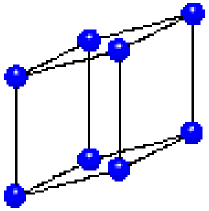


TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

P



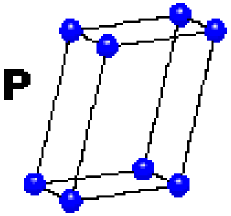
MONOCLINIC

$a \neq b \neq c$

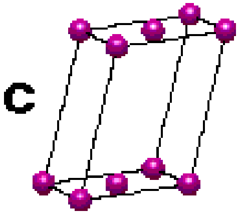
$\alpha = \gamma = 90°$

$\beta \neq 120°$

P



C

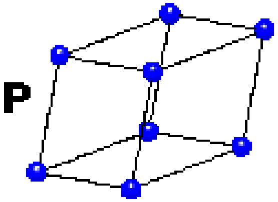


TRICLINIC

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$

P



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Coordinatıon Number

- Coordinatıon Number (CN) : The Bravais lattice points closest to a given point are the nearest neighbours.

- Because the Bravais lattice is periodic, all points have the same number of nearest neighbours or coordination number. It is a property of the lattice.

  - **A simple cubic has coordination number 6;**
  - **A body-centered cubic lattice, 8;**
  - **A face-centered cubic lattice,12.**

Atomic Packing Factor

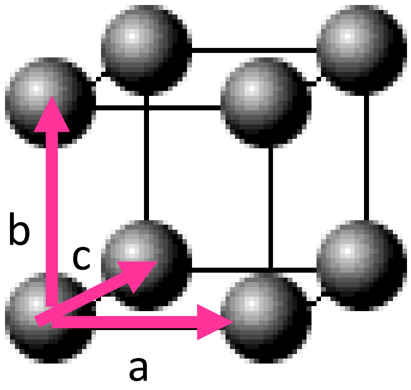
- Atomic Packing Factor (APF) is defined as the volume of atoms within the unit cell divided by the volume of the unit cell.

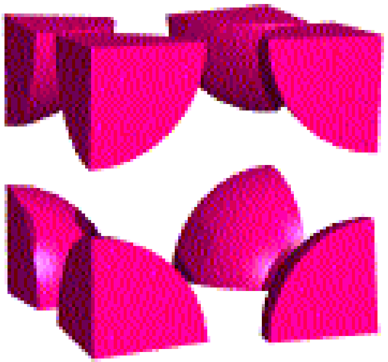
$$\text{APF} = \frac{\text{Volume of Atoms in Unit Cell}}{\text{Volume of Unit Cell}}$$

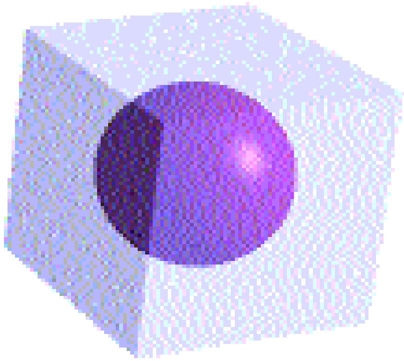
1-CUBIC CRYSTAL SYSTEM

a- Simple Cubic (SC)

- Simple Cubic has one lattice point so its primitive cell.
- In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) belongs to that cell. The rest of the atom belongs to neighboring cells.
- Coordinatination number of simple cubic is 6.







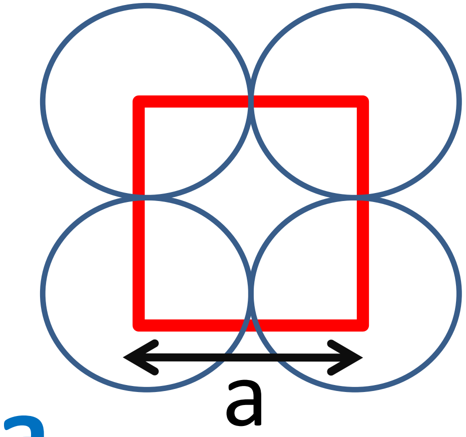
Atomic Radius for SC

- It is half the distance between any two nearest neighbors in the given crystal structure.
- It is expressed in terms of cube edge a

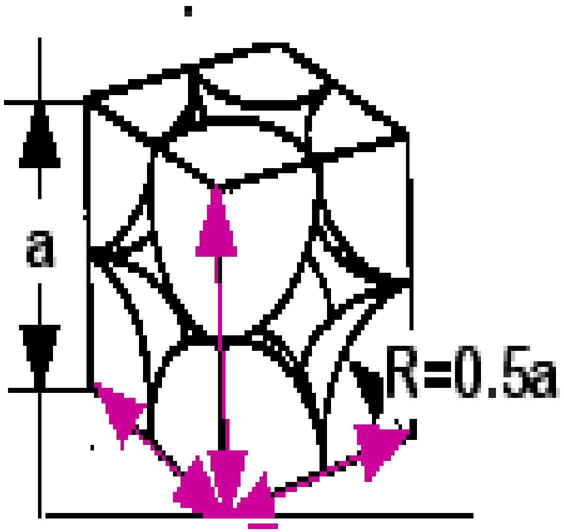
$a = 2r,$

$r = a/2$

Atomic Radius, $r = 0.5a$



Atomic Packing Factor of SC



APF = 0.52 for simple cubic

$$\frac{\text{atom}}{\text{unit cell}} \qquad \frac{\text{volume}}{\text{atom}}$$

$$\text{APF} = \frac{\boxed{1}\ \boxed{\frac{4}{3}\pi\,(0.5a)^3}}{\boxed{a^3}}$$

$$\frac{\text{volume}}{\text{unit cell}}$$

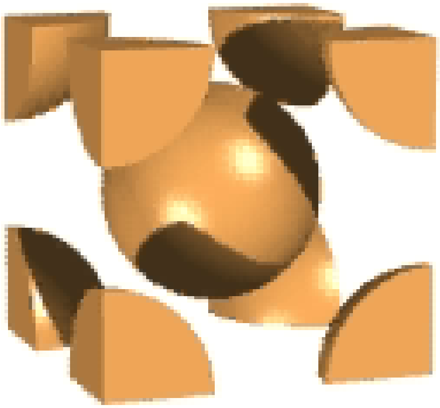
contains 8 x 1/8 =

1atom/unit cell

- APF = 0.52
- That means that the percentage of packing is 52%
- Thus, 52% of the volume of the simple cubic unit cell is occupied by atoms and the remaining 48% volume of unit cell is vacant or void space.

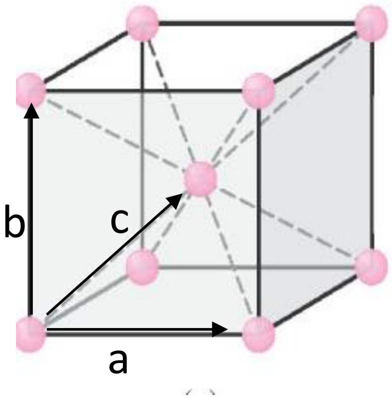
b-Body Centered Cubic (BCC)

- BCC structure has 8 corner atoms and 1 body centre atom.
- Each corner atom is shared by 8 unit cells.
- The center atom is not shared by any of the unit cells.
- So the



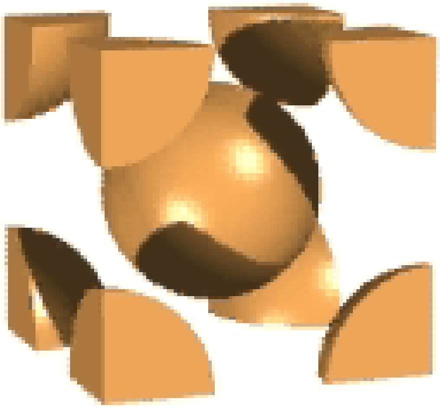
Number of atoms per unit cell

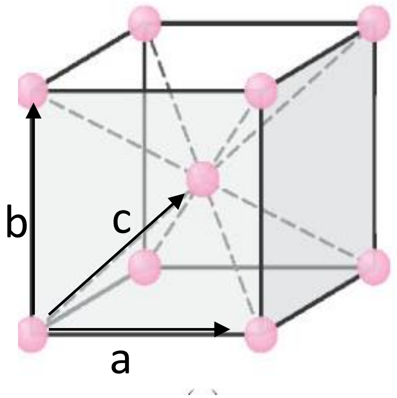
n = (1/8)x8 +1 = 2



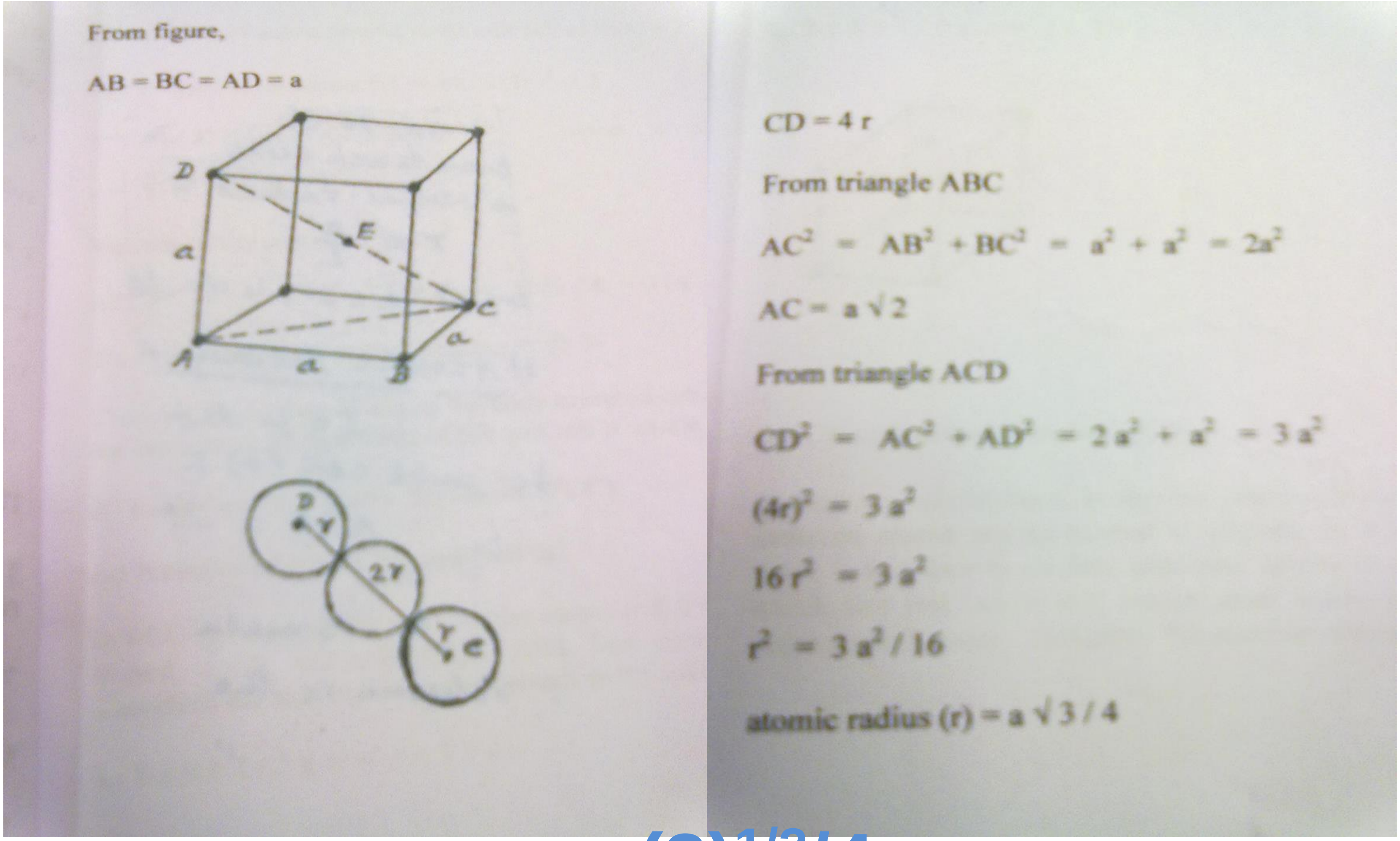
b-Body Centered Cubic (BCC)

- BCC has two lattice points so BCC is a non-primitive cell.
- BCC has eight nearest neighbors. Each atom is in contact with its neighbors only along the body-diagonal directions.
- **Hence, the coordination no. for BCC unit cell is 8**
- Many metals (Fe,Li,Na..etc), including the alkalis and several transition elements choose the BCC structure.





Atomic Radius for BCC unit cell



From figure,

AB = BC = AD = a

CD = 4 r

From triangle ABC

$AC^2 = AB^2 + BC^2 = a^2 + a^2 = 2a^2$

$AC = a\sqrt{2}$

From triangle ACD

$CD^2 = AC^2 + AD^2 = 2a^2 + a^2 = 3a^2$

$(4r)^2 = 3a^2$

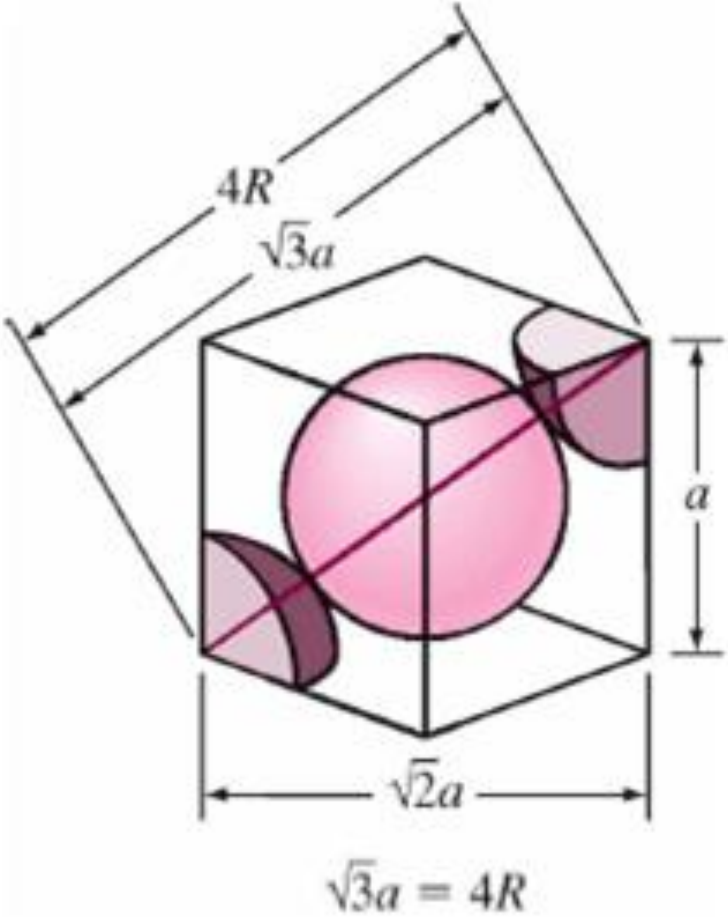
$16r^2 = 3a^2$

$r^2 = 3a^2 / 16$

atomic radius $(r) = a\sqrt{3} / 4$

$$r = a \times (3)^{1/2}/4$$

Atomic Packing Factor of BCC



$$APF_{BCC} = \frac{V_{atoms}}{V_{unit\ cell}} = 0.68$$

$$\frac{\text{atom}}{\text{unit cell}}$$

$$APF = \frac{\boxed{2}\ \boxed{\frac{4}{3}\ :(0,433a)^3}}{\boxed{a^3}}$$

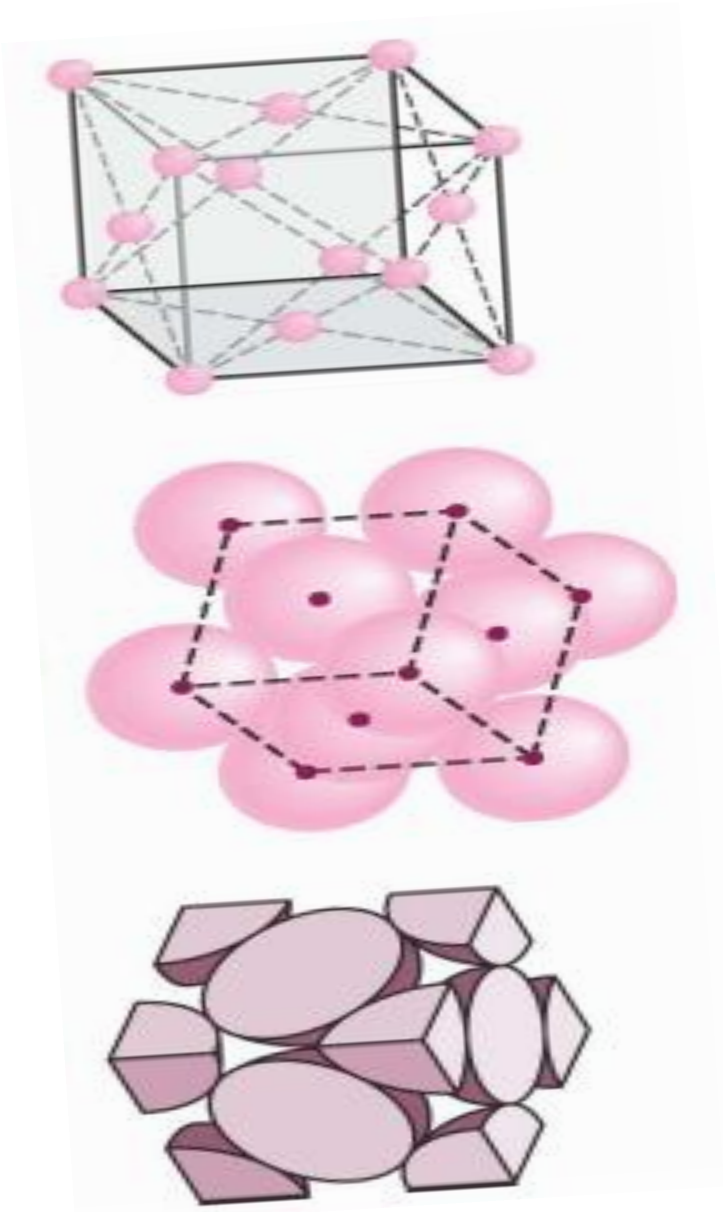
$$\frac{\text{volume}}{\text{atom}}$$

$$\frac{\text{volume}}{\text{unit cell}}$$

- The percentage of packing for BCC structure is 68%

- Thus , 68% of the volume of body centered cubic cell is occupied by atoms and the remaining 32% of the volume is vacant or void space

c- Face Centered Cubic (FCC)



- FCC structure has 8 corner atoms and 6 face centre atoms.
- Each corner atom is shared by 8 unit cells.
- Each face centered atom is shared by 2 unit cells.
- So the

Number of atoms present in unit cell is

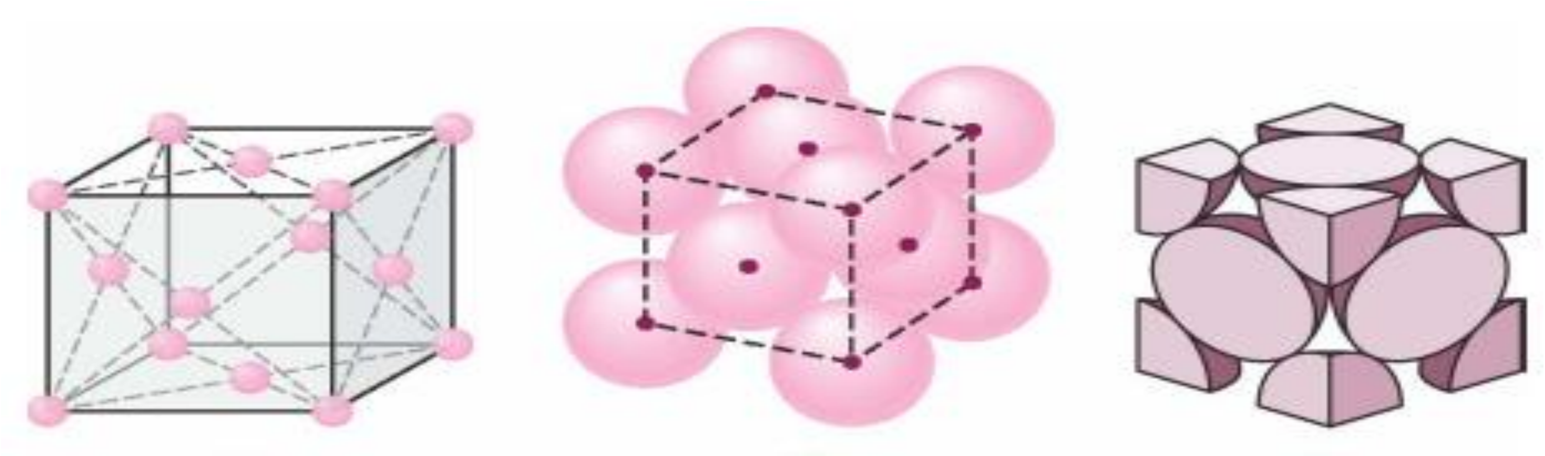
n = (1/8 x8) + (1/2 x 6)

= 1 + 3

= 4

- Co ordination Number
- The corner atom in its own plane touches 4 face centred atoms.
- In the plane just above, the corner atom has another 4 face centered atoms as its nearest neighbours
- Similarly, in the plane just below it has 4 more face centered atoms as its nearest neighbours
- Therefore the **no. of nearest neighbours are :**

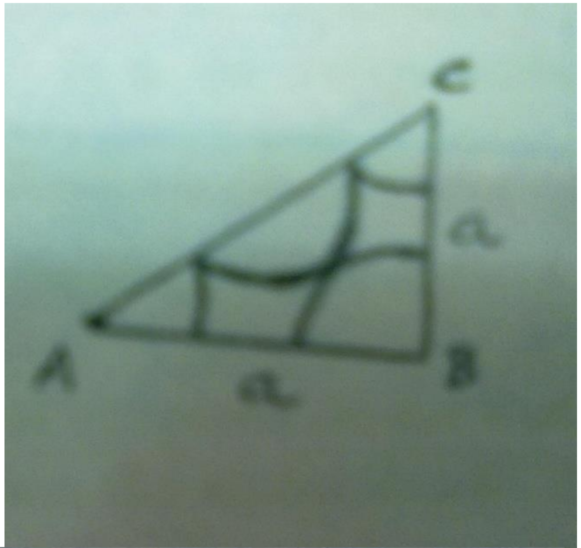
  4 + 4 + 4 = 12

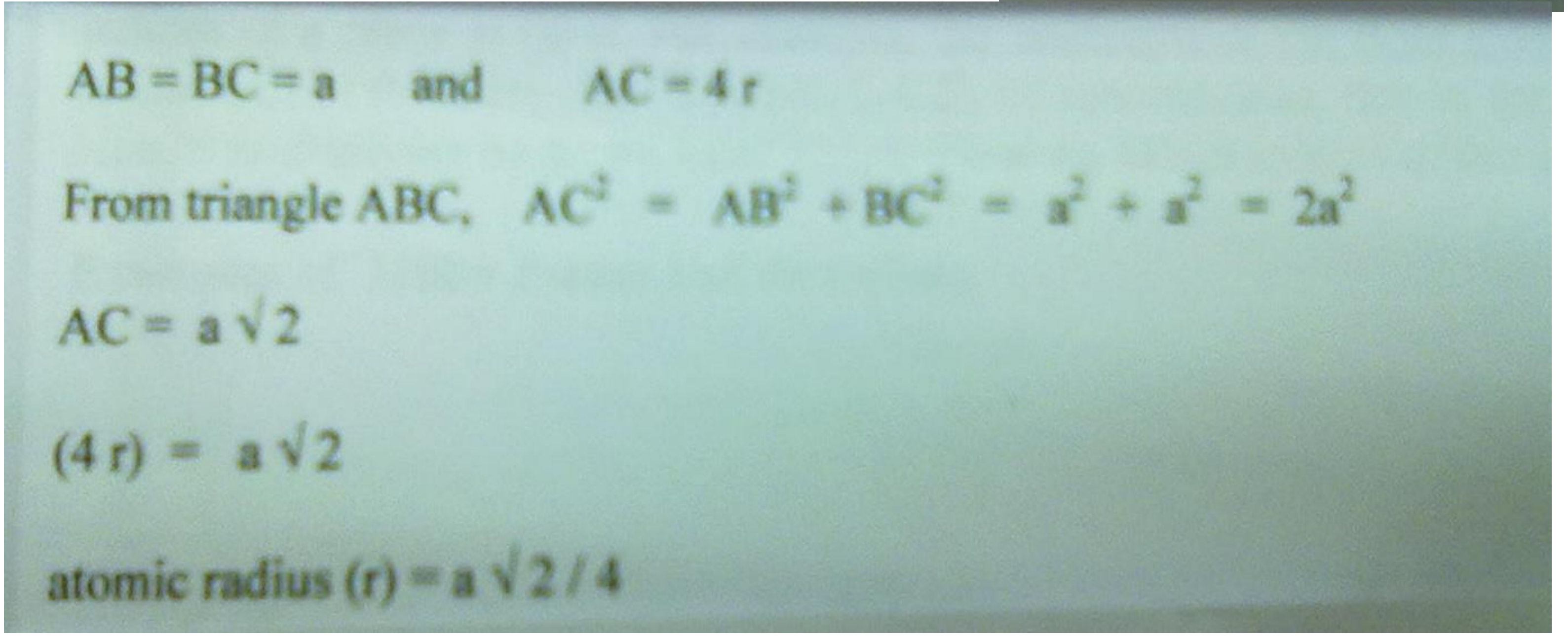


Many of common metals (Cu,Ni,Pb..etc) crystallize in FCC structure.

Atomic Radius for FCC

$r = a \times (2)^{1/2}/4$





$AB = BC = a$ and $AC = 4\,r$

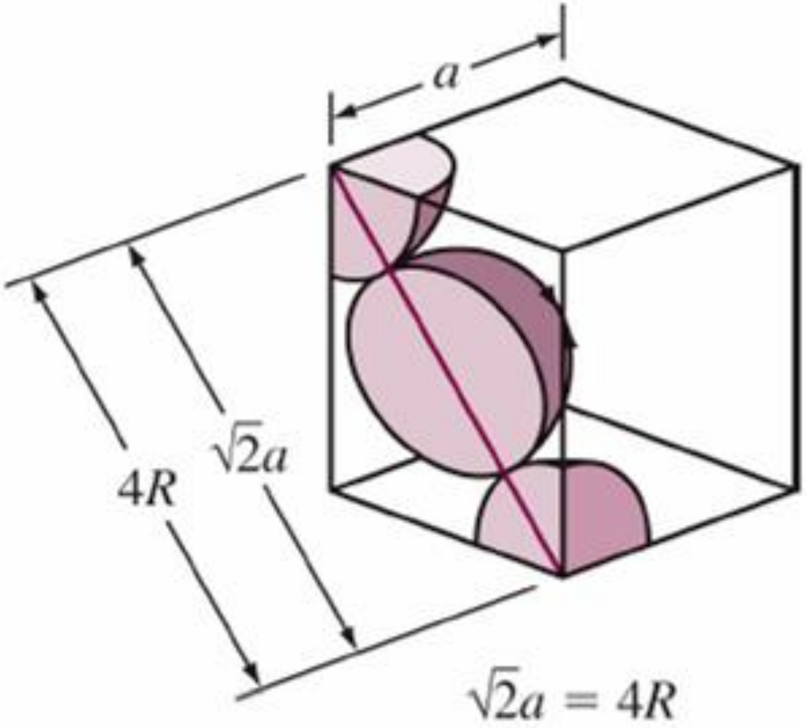
From triangle ABC, $AC^2 = AB^2 + BC^2 = a^2 + a^2 = 2a^2$

$AC = a\sqrt{2}$

$(4\,r) = a\sqrt{2}$

atomic radius $(r) = a\sqrt{2}/4$

Atomic Packing Factor of FCC



$$APF_{FCC} = \frac{V_{atoms}}{V_{unit\ cell}} = 0.74$$

$$\frac{\text{atom}}{\text{unit cell}}$$

$$\frac{\text{volume}}{\text{atom}}$$

$$APF = \frac{\boxed{4}\ \boxed{\frac{4}{3}\pi(0.353a)^3}}{\boxed{a^3}}$$

$$\frac{\text{volume}}{\text{unit cell}}$$

Unit cell contents

Counting the number of atoms within the unit cell

Atoms	Shared Between:	Each atom counts:
corner	8 cells	1/8
face centre	2 cells	1/2
body centre	1 cell	1

lattice type	cell contents	
P	1	[=8 x 1/8]
I	2	[=(8 x 1/8) + (1 x 1)]
F	4	[=(8 x 1/8) + (6 x 1/2)]

Crystal Directions

- **We choose one lattice point on the line as an origin, say the point O. Choice of origin is completely arbitrary, since every lattice point is identical.**
- **Then we choose the lattice vector joining O to any point on the line, say point T. This vector can be written as;**

$$R = n_1 a + n_2 b + n_3 c$$

- **To distinguish a lattice <u>direction</u> from a lattice <u>point</u>, the triple is enclosed in square brackets [...] is used.[$n_1 n_2 n_3$]**
- **[$n_1 n_2 n_3$] is the <u>smallest integer</u> of the <u>*same relative ratios*</u>.**

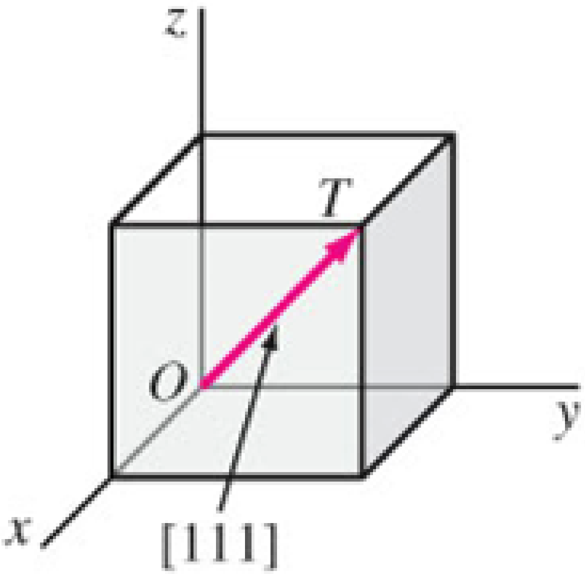
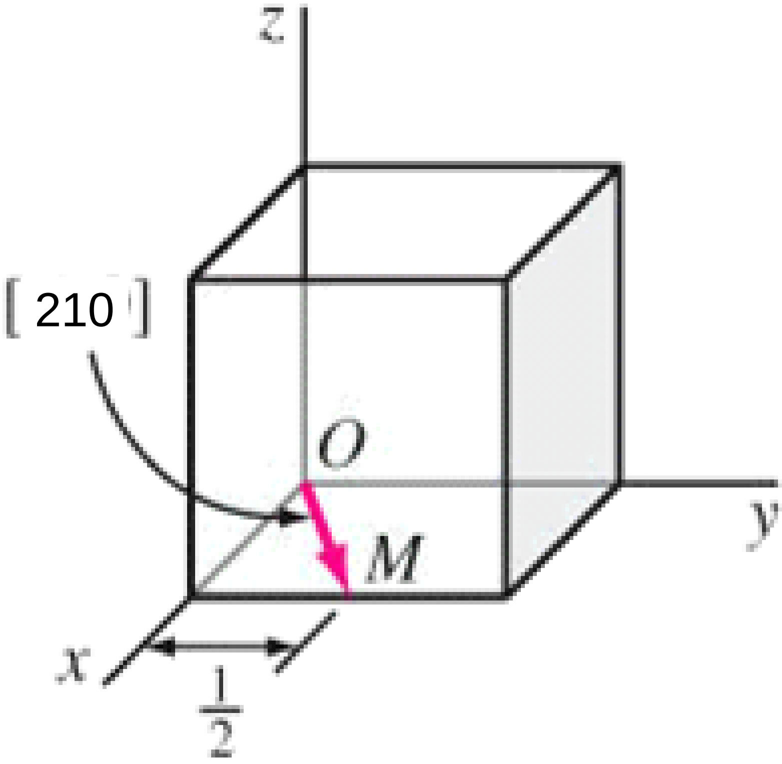
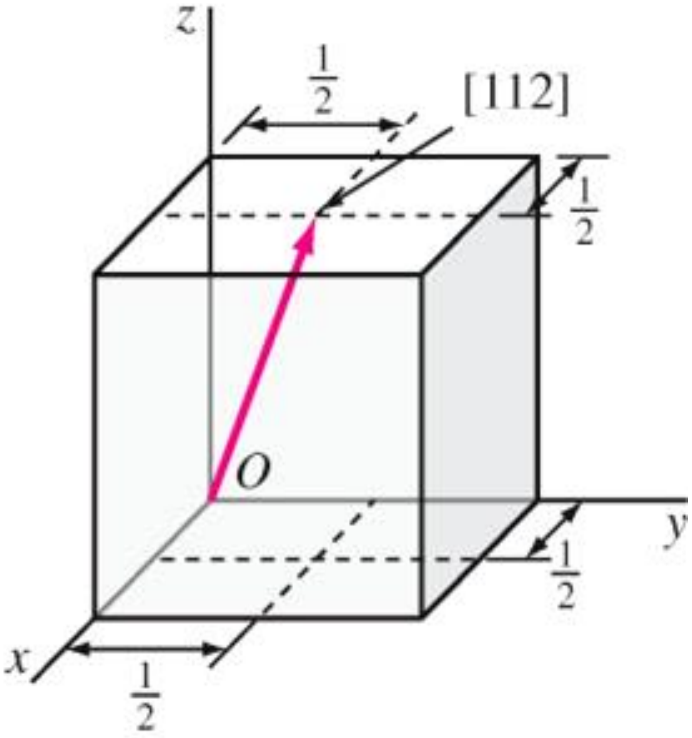


Fig. Shows [111] direction

Examples



X = 1 , Y = ½ , Z = 0
[1 ½ 0] ⇨ [2 1 0]



X = ½ , Y = ½ , Z = 1
[½ ½ 1] ⇨ [1 1 2]

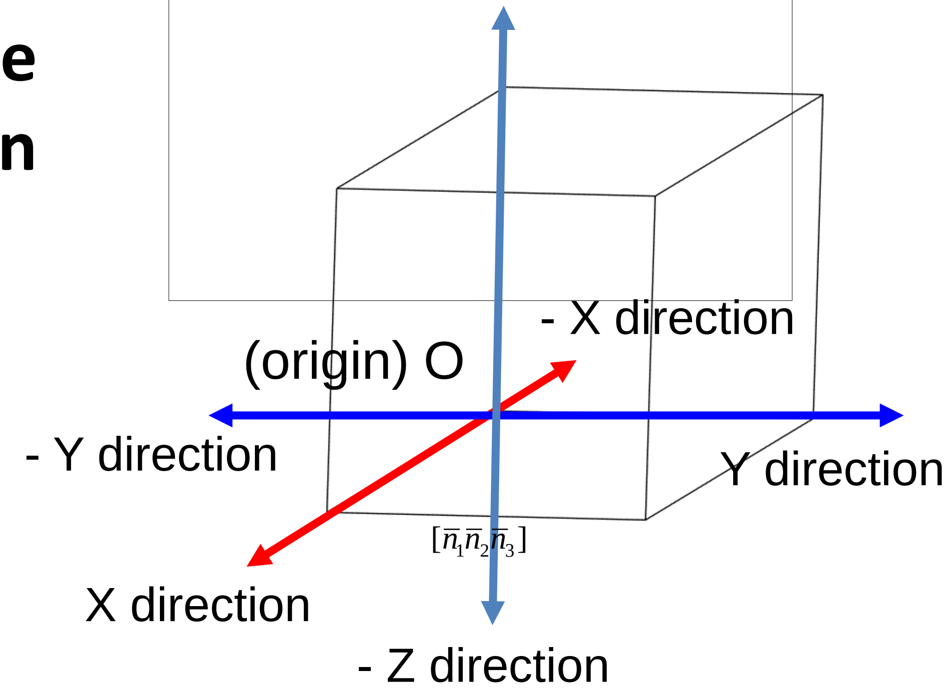
Negative directions

- **When we write the direction $[n_1n_2n_3]$ depend on the origin, negative directions can be written as**

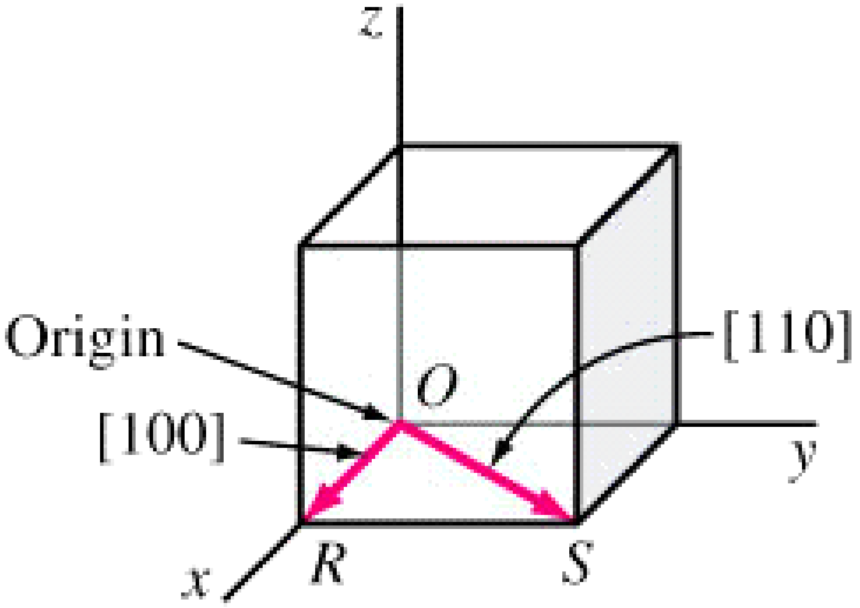
$$[\bar{n}_1\bar{n}_2\bar{n}_3]$$

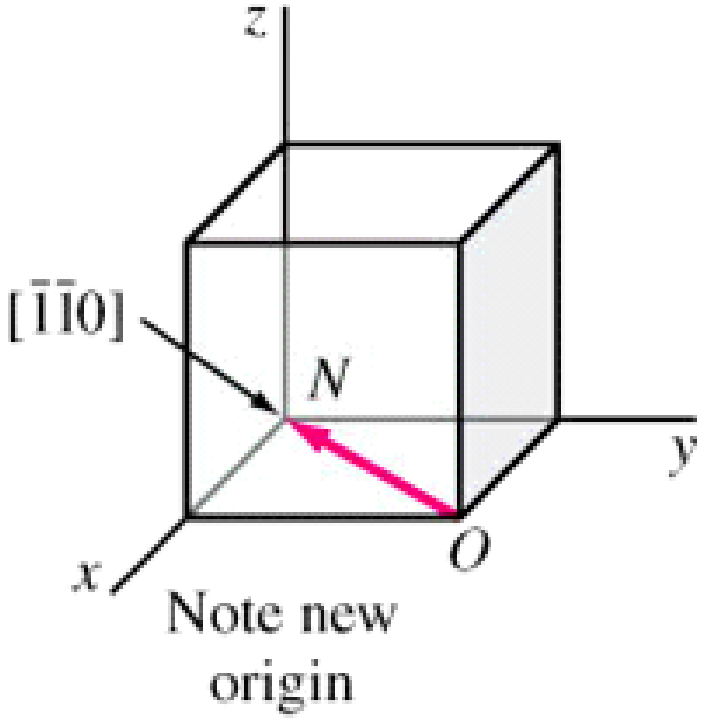
- **$R = n_1\,a + n_2\,b + n_3c$**

Direction must be smallest integers.



Examples of crystal directions

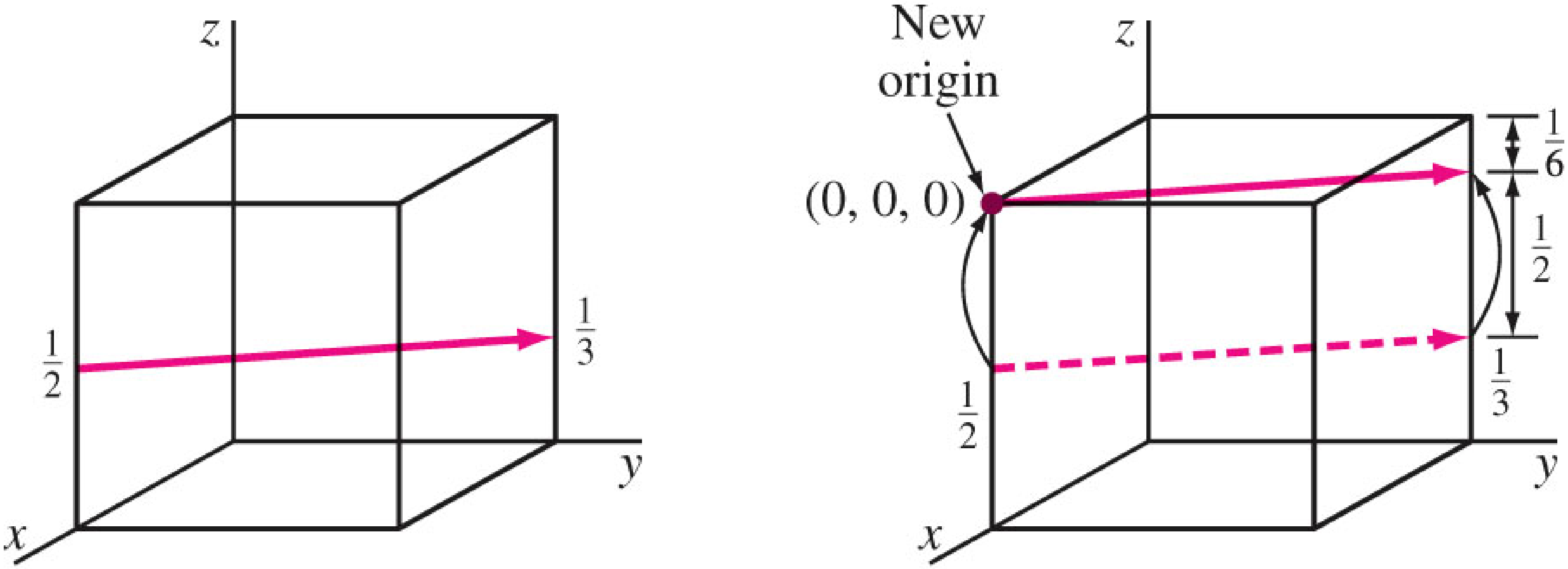




X = 1 , Y = 0 , Z = 0 ⇨ [1 0 0]

X = -1 , Y = -1 , Z = 0 ⇨ $[\overline{11}0]$

Examples



(a)

(b)

We can move vector to the origin.

X =-1 , Y = 1 , Z = -1/6

[-1 1 -1/6] ⇨ $[\bar{6}\ 6\ \bar{1}]$

Symmetry Element of a Crystalline Solids

- Axis of symmetry
- Plane of Symmetry
- Centre of Symmetry

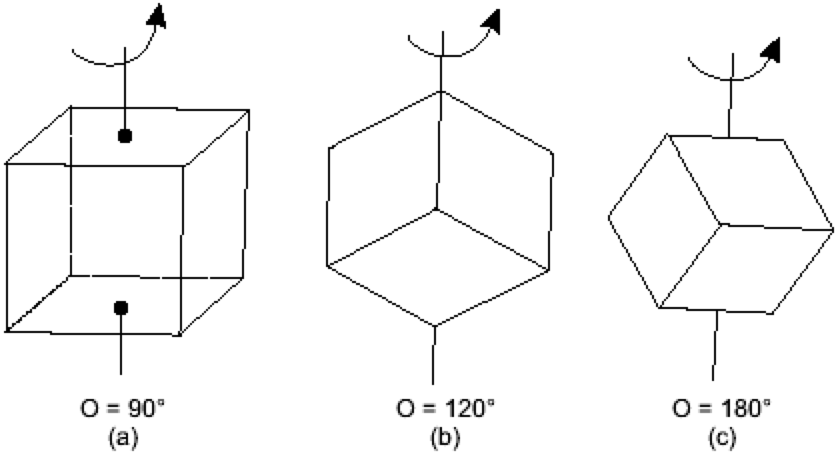
There are 13 axes of symmetry for a cube

- Three axes have four fold symmetry know as tetrad. These axes pass through opposite face centres.
- Four axes have three fold symmetry know as triad. These axes pass through diagonally opposite corners.
- Six axes have two fold symmetry know as diad. These axes pass through the centers of opposite edges.

SYMMETRY ELEMENT OF A CRYSTALLINE SOLID

Axis of Symmetry

- 3 axes have four-fold symmetry known as *tetrad*. *These axes pass through opposite face centres.*
- 4 axes have three-fold symmetry known as *triad*. *These axes pass through diagonally opposite* corners.
- 6 axes have two-fold symmetry known as *diad*. *These axes pass through the centres of opposite* edges.



(a) 4-fold axes of symmetry, **(b)** 3-fold axes of symmetry, and **(c)** 2-fold axes of symmetry

Planes of Symmetry

- If a plane is able to cut a crystal into two halves in such a way that one half becomes the mirror image of the other half then the plane is known as plane of symmetry.

- There are 9 such planes

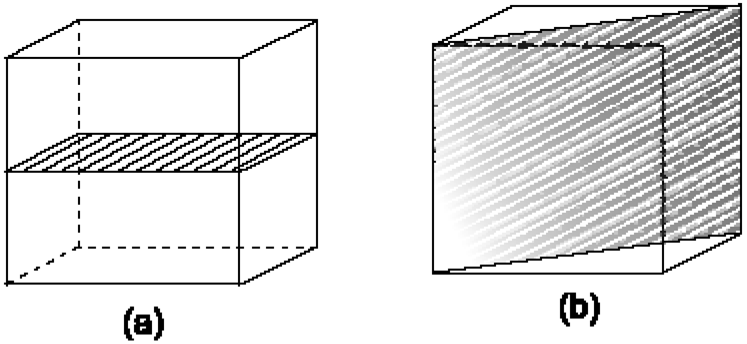
- 3 are parallel to the faces of the cube.

- 6 are diagonal planes passing through diagonally opposite parallel edges.

Planes of Symmetry

- If a plane is able to cut a crystal into two halves in such a way that one half becomes the mirror image of the other half, then that plane is known as the plane of symmetry.

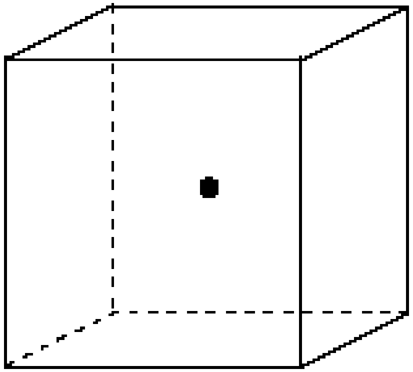
- There are 9 planes—3 are parallel to the face of the cube and 6 are diagonal planes passing through diagonally opposite parallel edges.



(a) Parallel plane of symmetry and **(b)** diagonal plane of symmetry

Centre of Symmetry

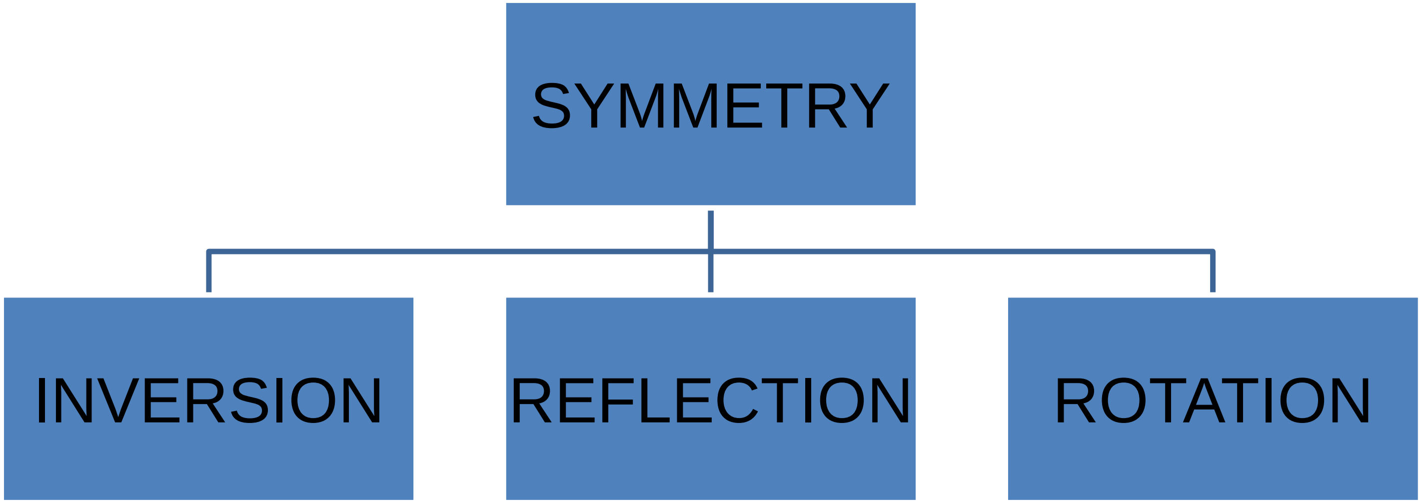
- It is defined as a point in a crystal such that if a line is drawn from any point in the crystal through the point and an equal distance is produced on the other side of this central point, then it meets an identical point. There is only one centre of symmetry for cube system.



Centre of symmetry in cubic system

ELEMENTS OF SYMMETRY

- Each of the unit cells of the 14 Bravais lattices has one or more types of symmetry properties, such as inversion, reflection or rotation,etc.



SYMMETRY

INVERSION

REFLECTION

ROTATION

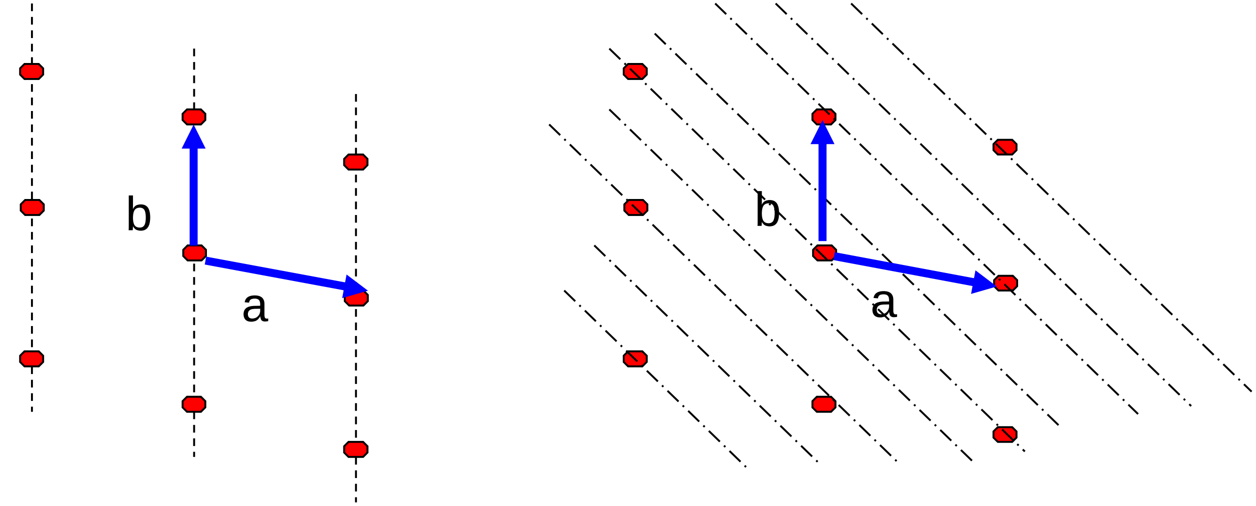
Lattice goes into itself through Symmetry without translation

Operation	Element
Inversion	Point
Reflection	Plane
Rotation	Axis
Rotoinversion	Axes

Crystal Planes

- Within a crystal lattice it is possible to identify sets of equally spaced parallel planes. These are called lattice planes.
- In the figure density of lattice points on each plane of a set is the same and all lattice points are contained on each set of planes.

The set of planes in 2D lattice.



Miller Indices

Miller Indices are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals of the fractional intercepts which the plane makes with the crystallographic axes.

To determine Miller indices of a plane, take the following steps;

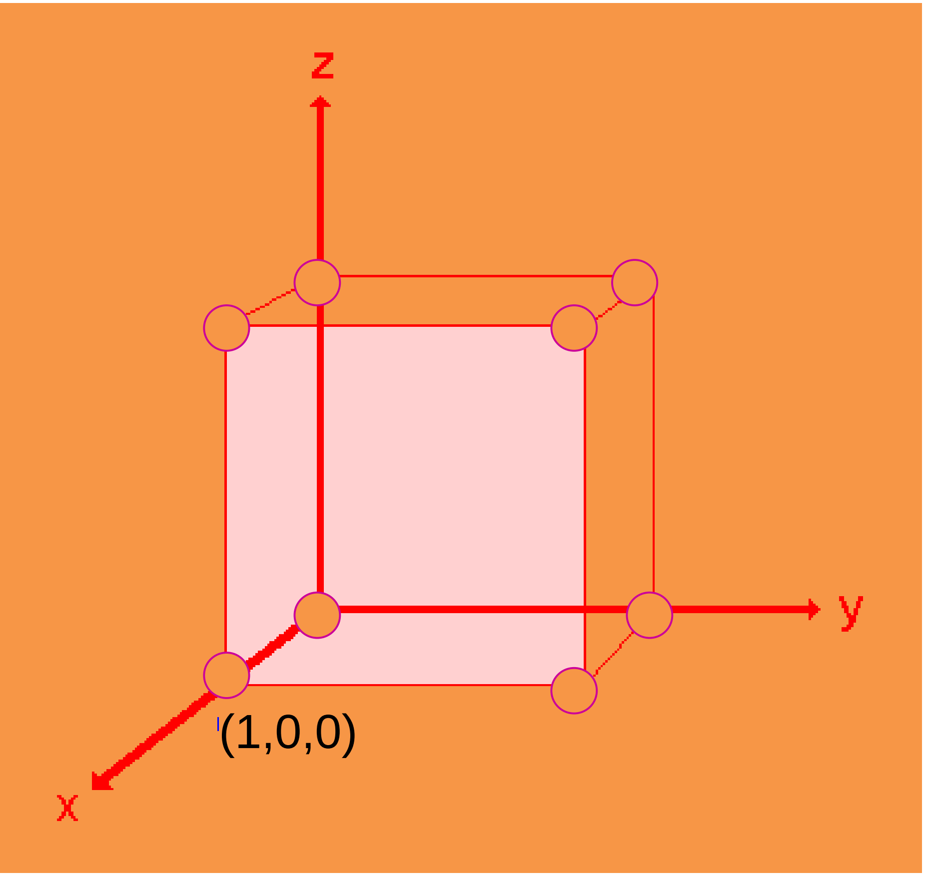
1. Choose a system of three coordinate axes , preferabally along the crstallographic axes.
2. Determine the intercepts of the plane along each of the three crystallographic directions usually along the coordinate axes x,y,z.

3. Express these intercepts in the terms of axial unit.
4. Take the reciprocals of the intercepts.

5. Taking LCM of numerical values of above intercepts , reduce them to the smallest three integers which have same ratio.

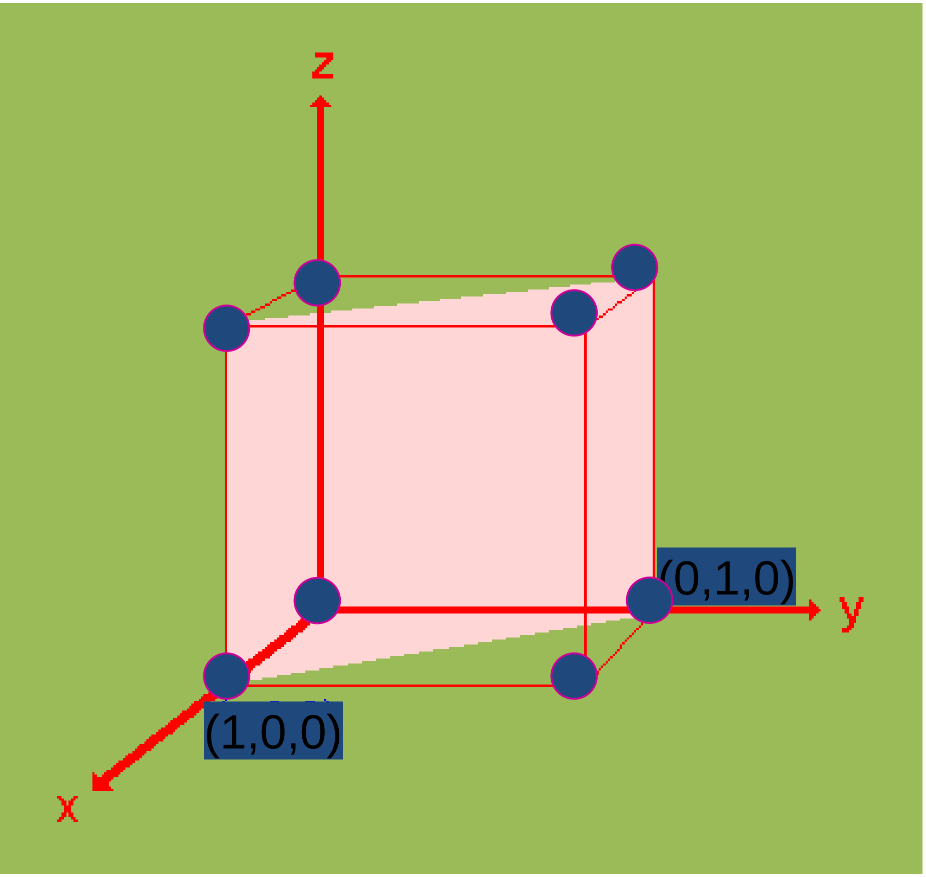
6. Enclose the result of obtain in step-5 in the parentheses (hkl), which are known as Miller indices of the crystal plane.

Example-1



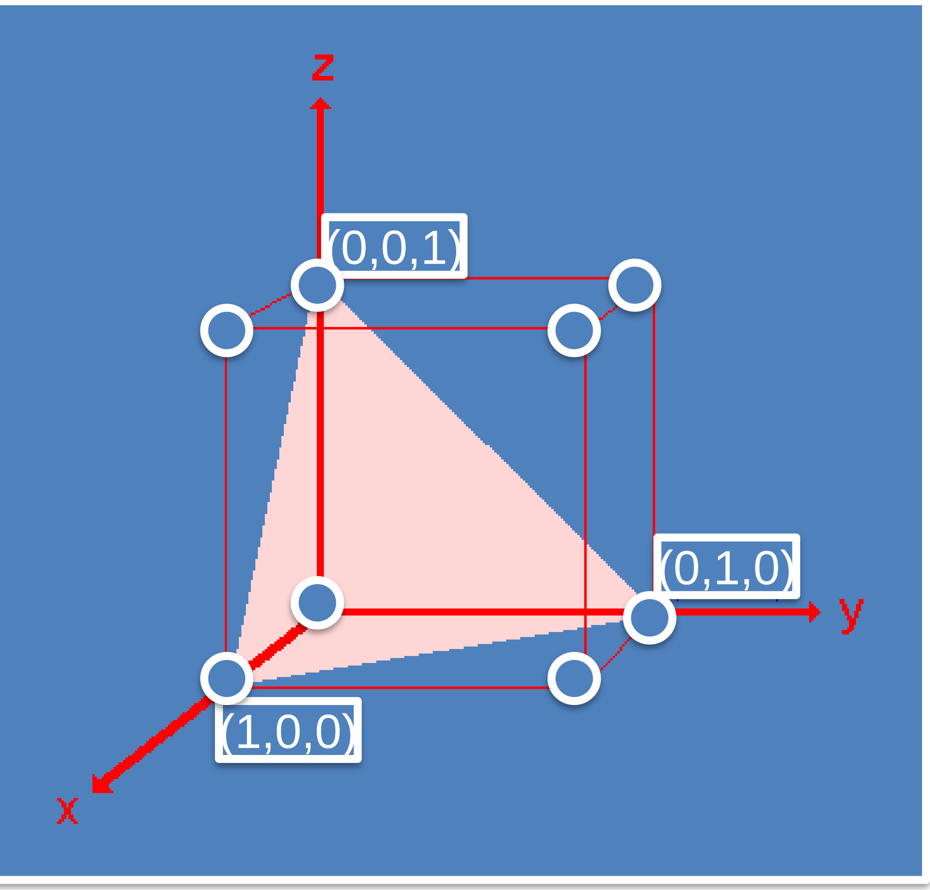
Axis	X	Y	Z
Intercept points	1	∞	∞
Reciprocals	1/1	1/ ∞	1/ ∞
Smallest Ratio	1	0	0
Miller İndices (100)			

Example-2



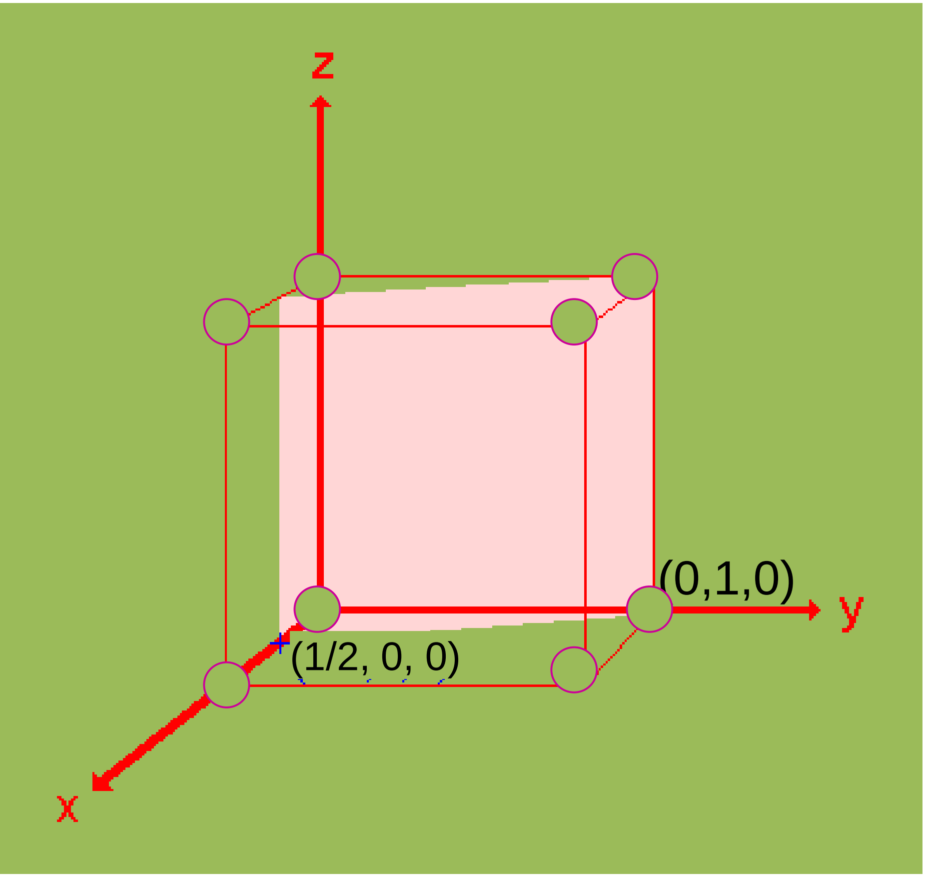
Axis	X	Y	Z
Intercept points	1	1	∞
Reciprocals	1/1	1/ 1	1/ ∞
Smallest Ratio	1	1	0
Miller İndices (110)			

Example-3



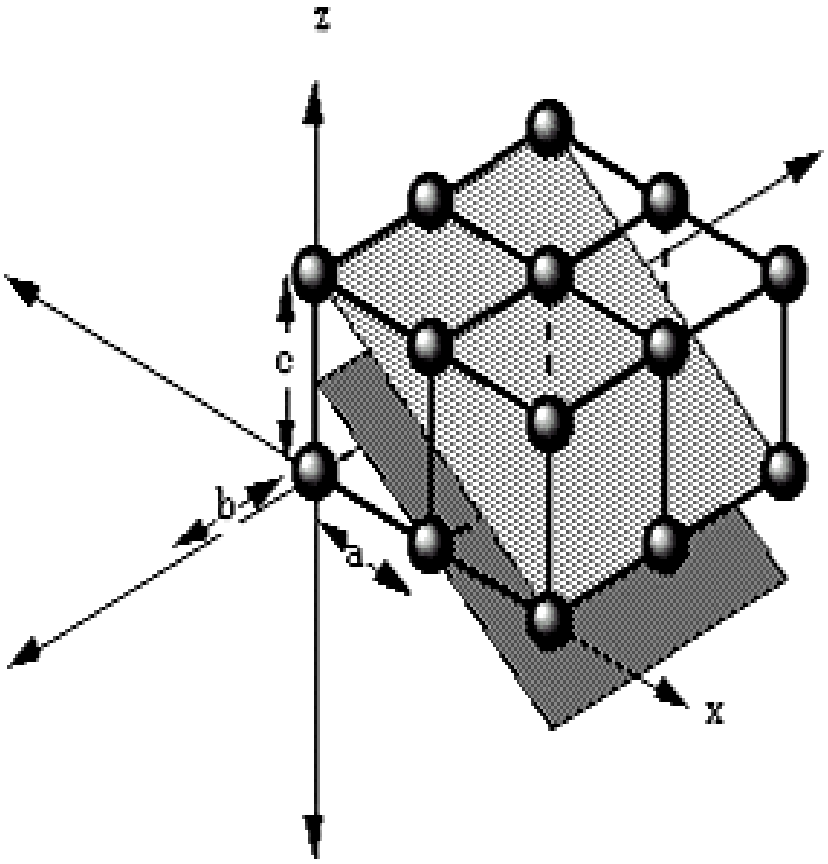
Axis	X	Y	Z
Intercept points	1	1	1
Reciprocals	1/1	1/ 1	1/ 1
Smallest Ratio	1	1	1
Miller İndices (111)			

Example-4



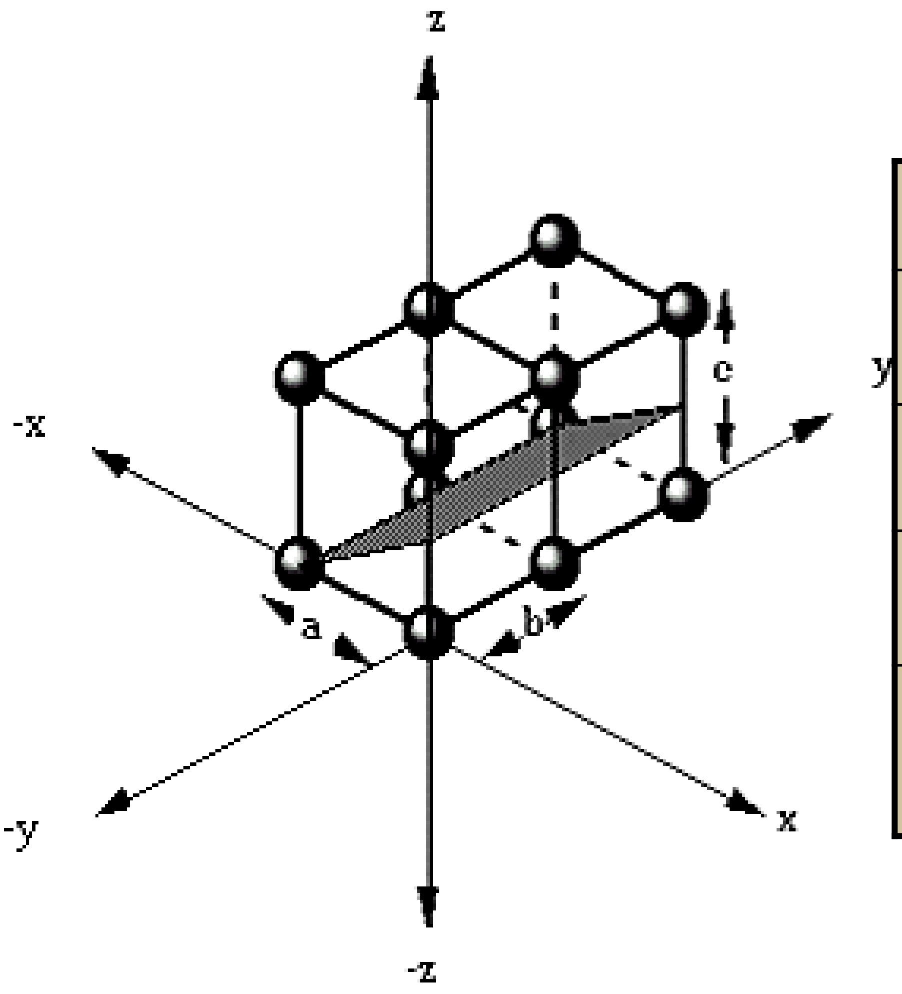
Axis	X	Y	Z
Intercept points	1/2	1	∞
Reciprocals	1/(½)	1/ 1	1/ ∞
Smallest Ratio	2	1	0
Miller İndices (210)			

Example-5



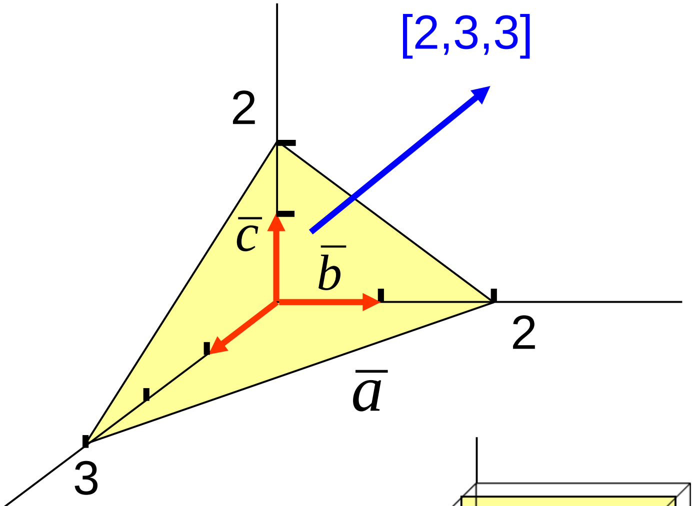
Axis	a	b	c
Intercept points	1	∞	½
Reciprocals	**1/1**	**1/ ∞**	**1/(½)**
Smallest Ratio	1	0	2
Miller İndices (102)			

Example-6



Axis	a	b	c
Intercept points	-1	∞	½
Reciprocals	**1/-1**	**1/ ∞**	**1/(½)**
Smallest Ratio	-1	0	2
Miller İndices $(\bar{1}02)$			

Miller Indices

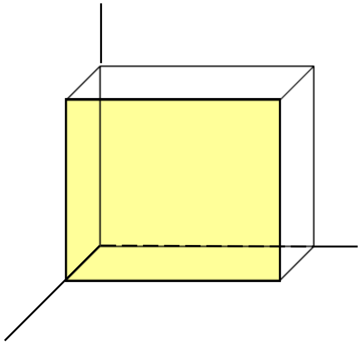


Plane intercepts axes at $3\bar{a}, 2\bar{b}, 2\bar{c}$

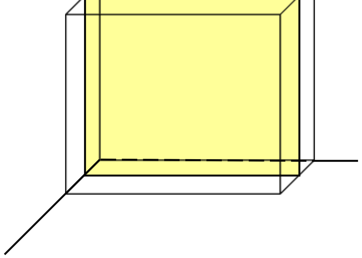
Reciprocal numbers are: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

Indices of the plane (Miller): (2,3,3)

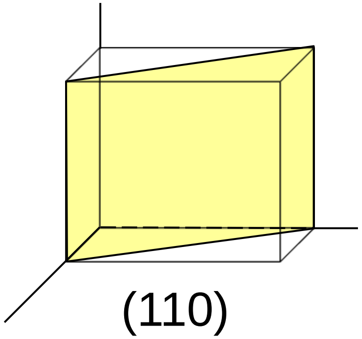
Indices of the direction: [2,3,3]



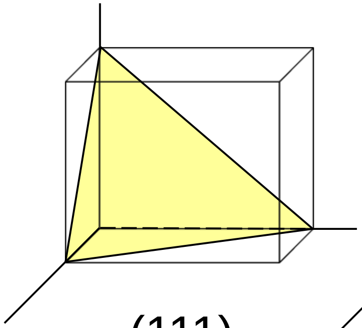
(100)



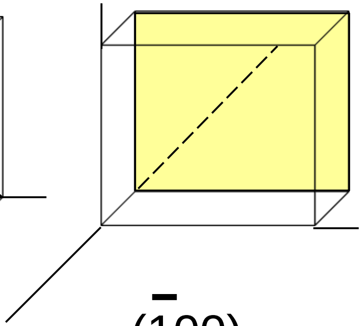
(200)



(110)

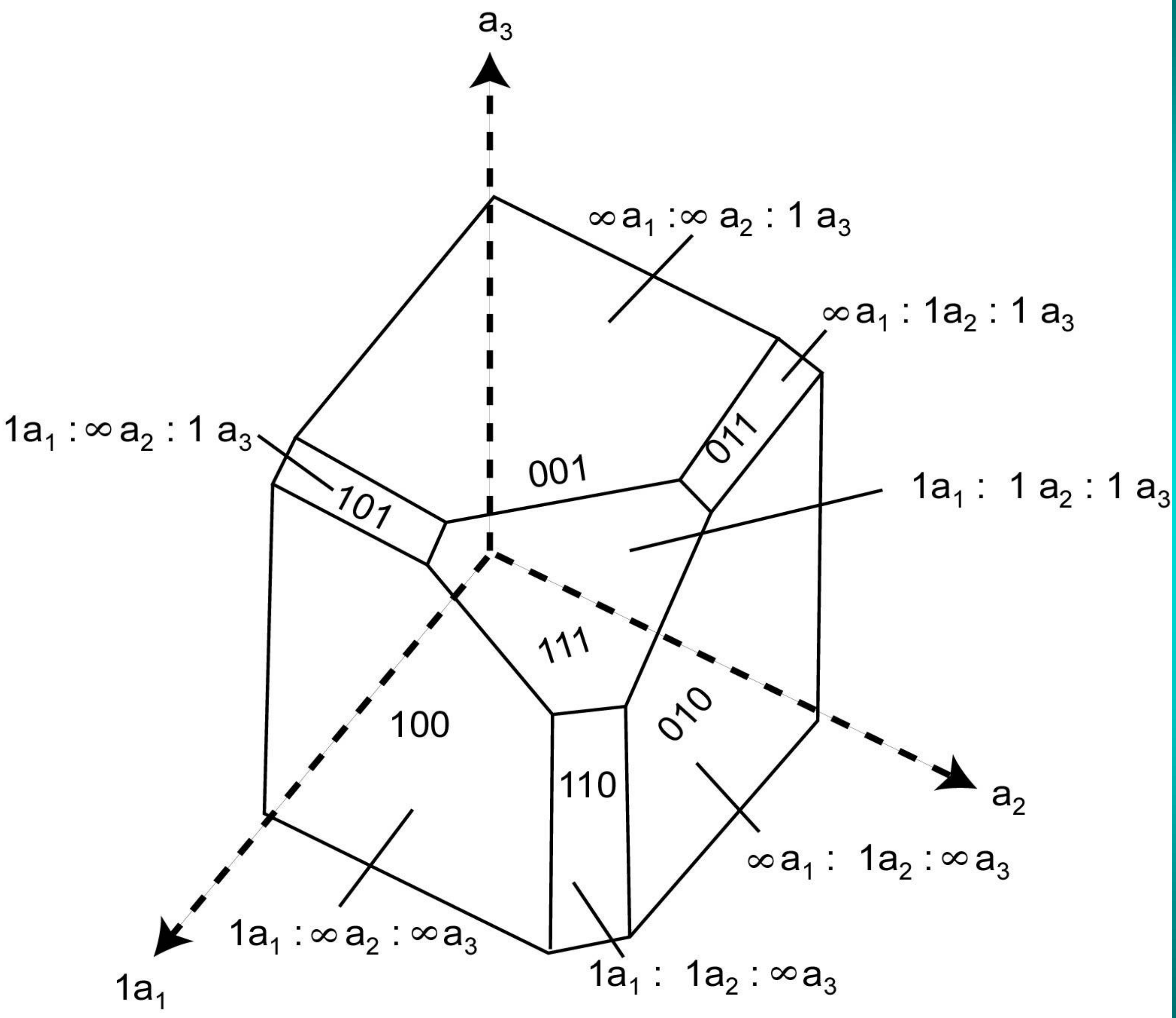


(111)

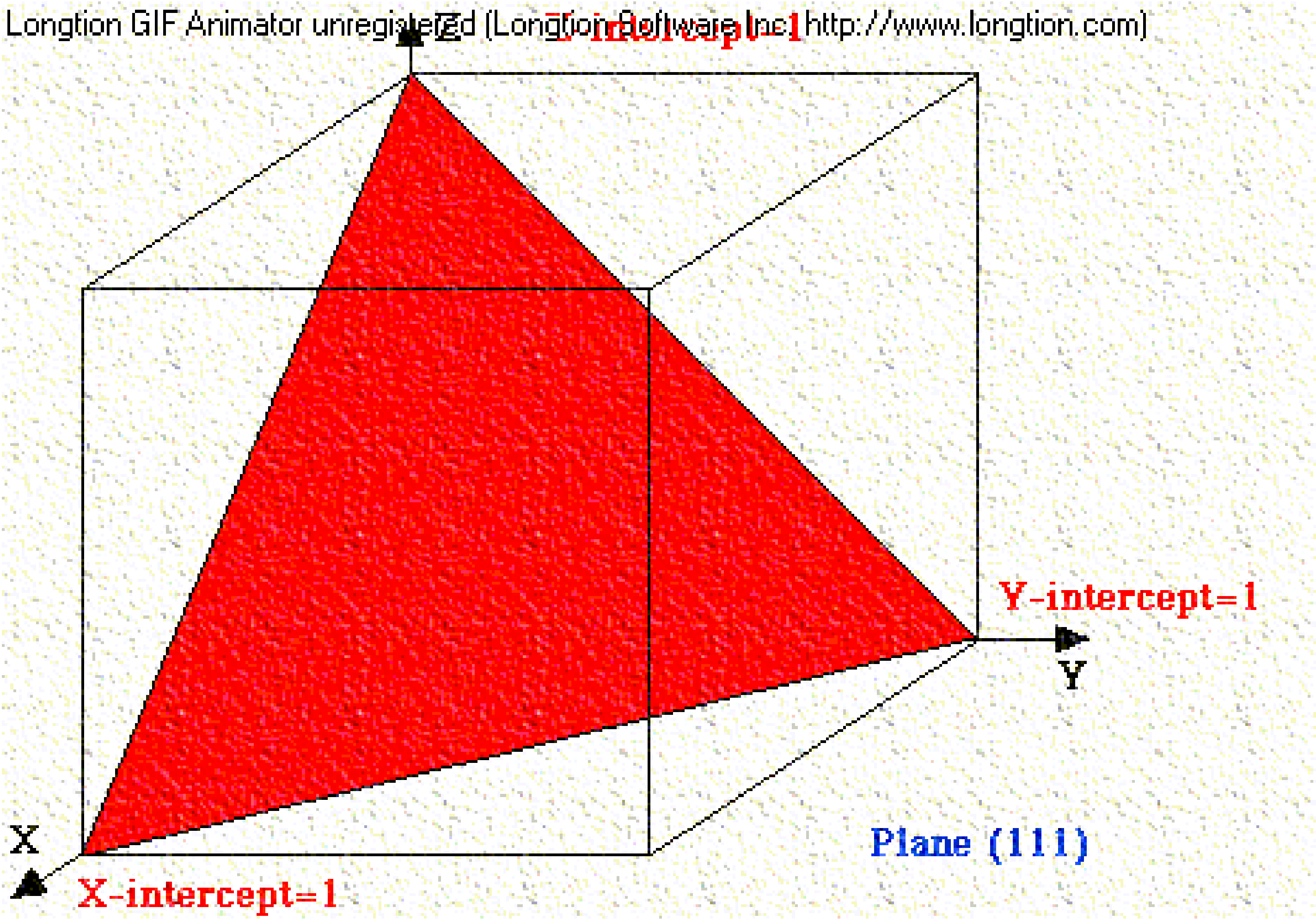


$(\bar{1}00)$

Miller indices and intercepts



Example-7

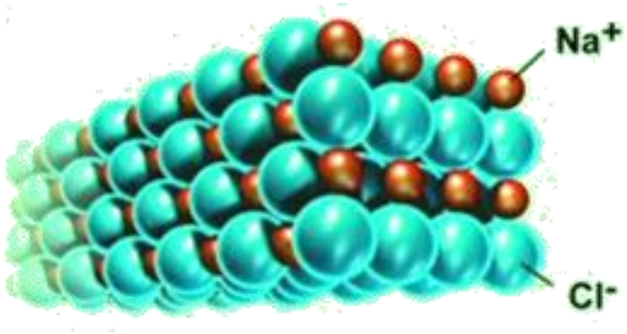


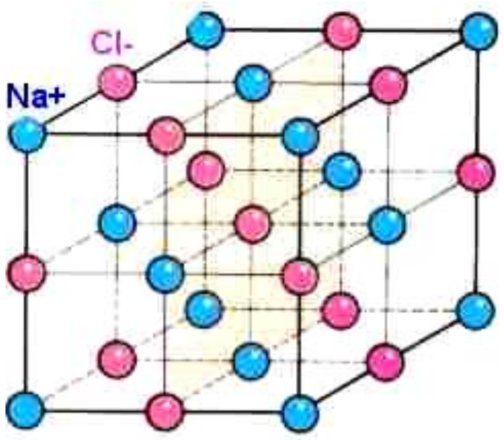
THE MOST IMPORTANT CRYSTAL STRUCTURES

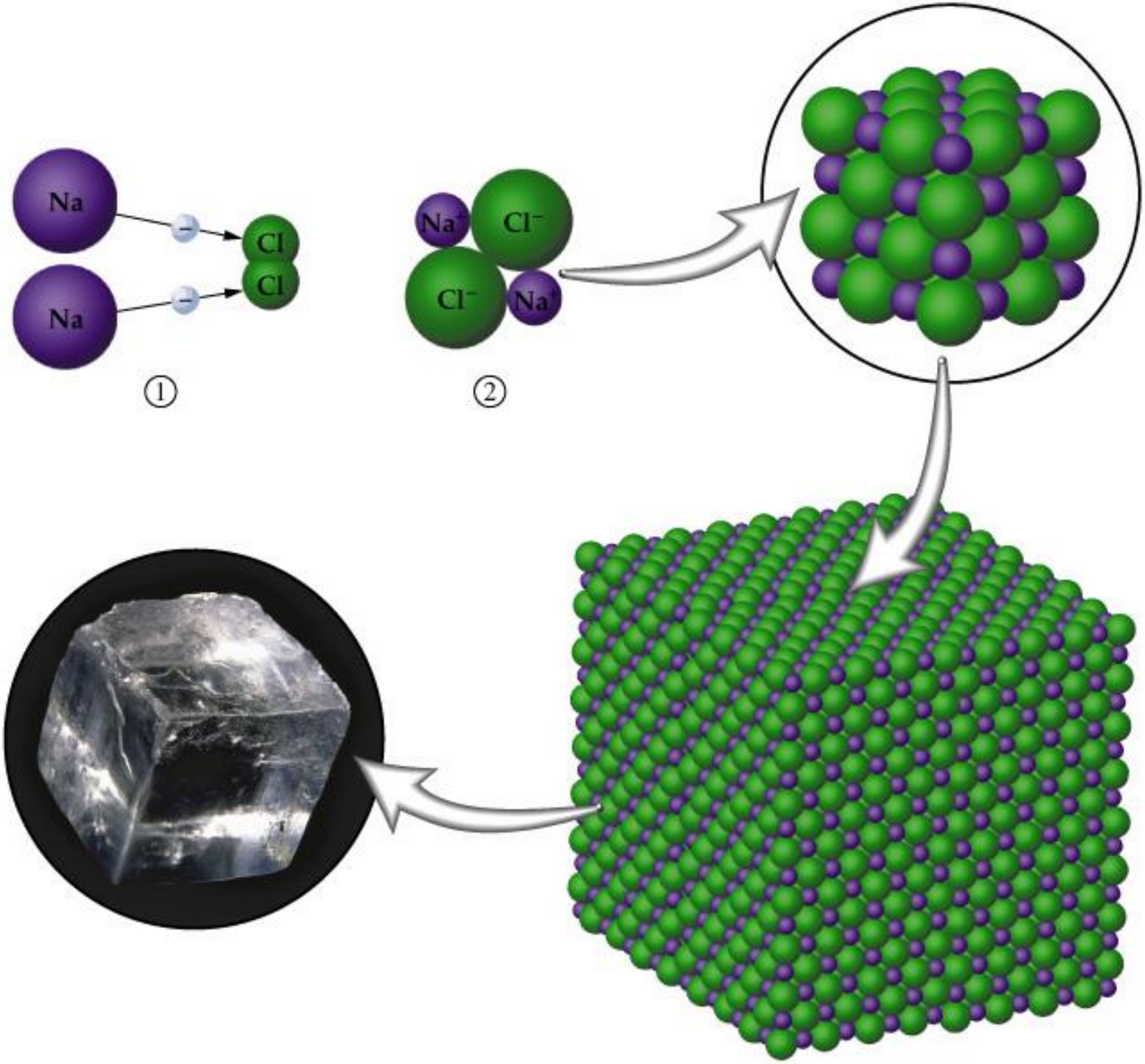
- Sodium Chloride Structure Na^+Cl^-
- Cesium Chloride Structure Cs^+Cl^-
- Hexagonal Closed-Packed Structure
- Diamond Structure
- Zinc Blende

1 – Sodium Chloride Structure

- **Sodium chloride also crystallizes in a cubic lattice, but with a different unit cell.**
- **Sodium chloride structure consists of equal numbers of sodium and chlorine ions placed at alternate points of a simple cubic lattice.**
- **Each ion has six of the other kind of ions as its nearest neighbours.**

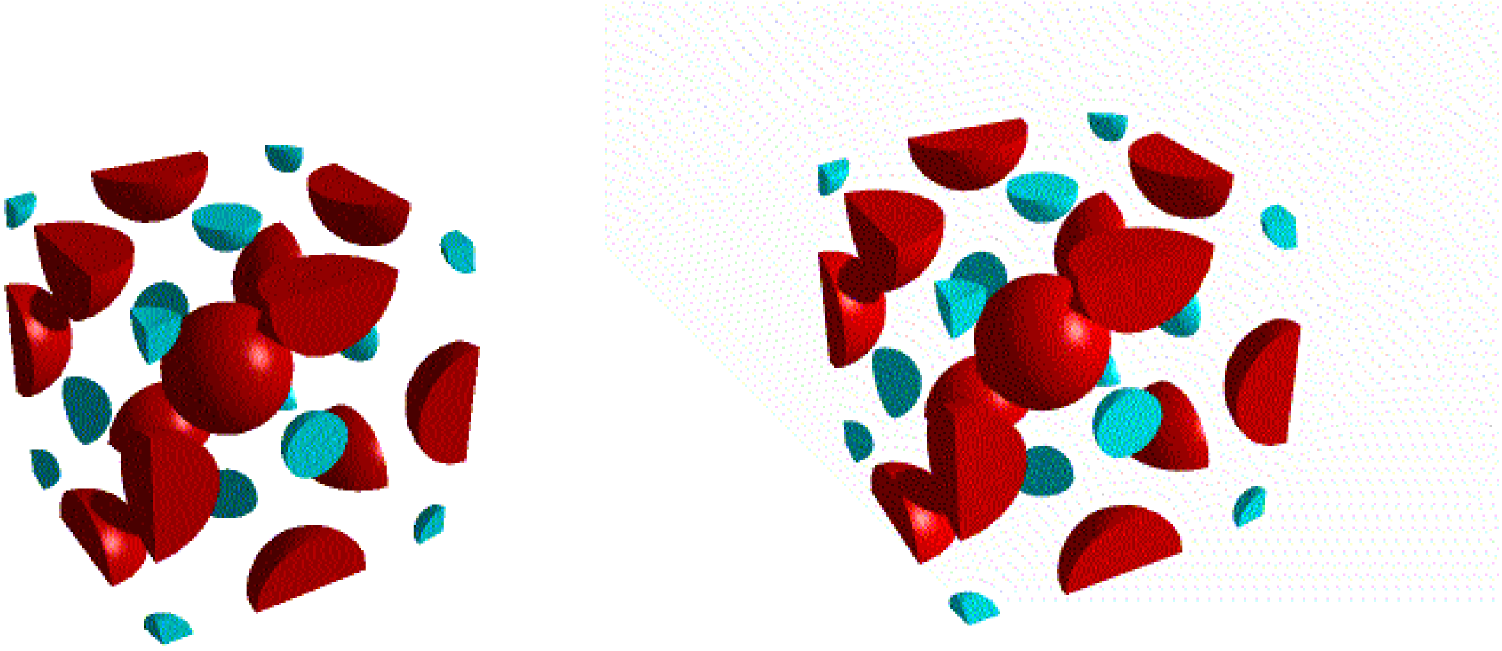




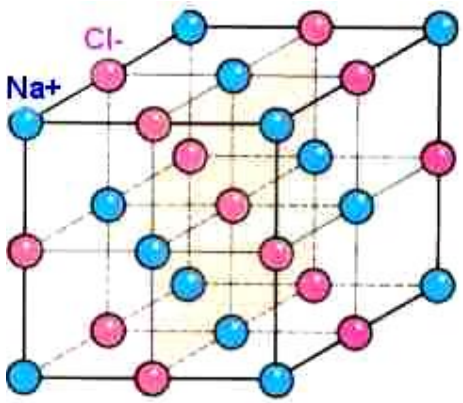

Na
−
Cl
Cl
Na
−
①
Na+
Cl−
Cl−
Na+
②

Sodium Chloride Structure

- **If we take the NaCl unit cell and remove all the red Cl ions, we are left with only the blue Na. If we compare this with the fcc unit cell, it is clear that they are identical. Thus, the Na is in a fcc sublattice.**



Sodium Chloride Structure



- This structure can be considered as a face-centered-cubic Bravais lattice with a basis consisting of a sodium ion at 0 and a chlorine ion at the center of the conventional cell,

$$a/2(\vec{x}+\vec{y}+\vec{z})$$

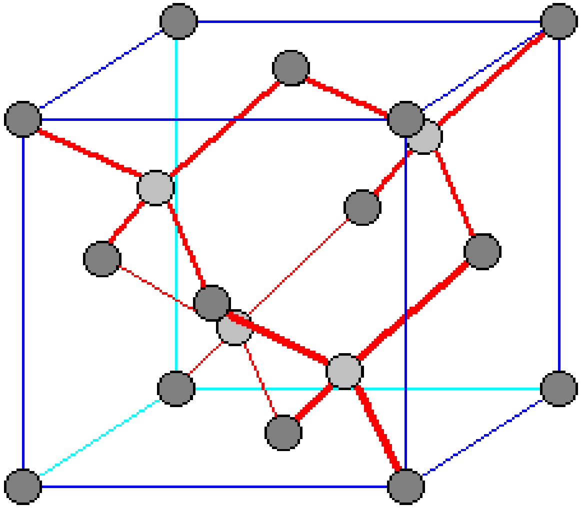
- LiF,NaBr,KCl,LiI,etc
- The lattice constants are in the order of 4-7 angstroms.

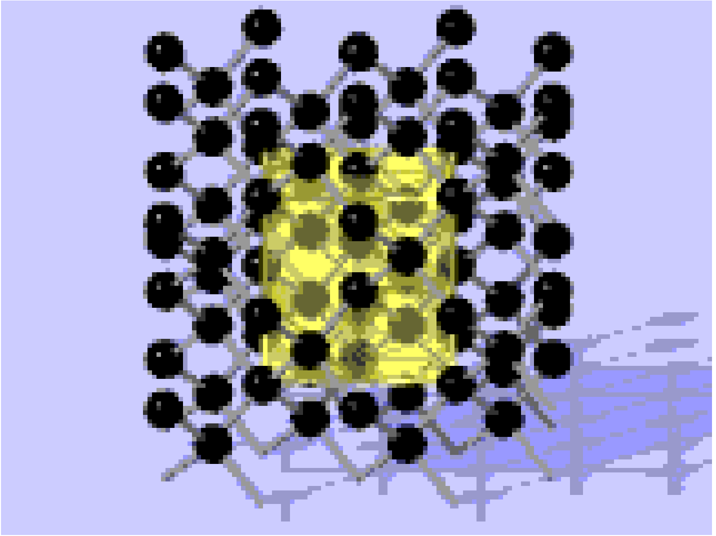
4 - Diamond Structure

- The coordination number of diamond structure is 4.
- The diamond lattice is not a Bravais lattice.
- Si, Ge and C crystallizes in diamond structure.

4 - Diamond Structure

- **The diamond lattice is consist of two interpenetrating face centered bravais lattices.**
- **There are eight atom in the structure of diamond.**
- **Each atom bonds covalently to 4 others equally spread about atom in 3d.**





Reciprocal Lattice

- The concepts of reciprocal lattice, structure factor calculations (and sometimes Ewald sphere construction) often ‘strike terror’ in the hearts of students.
- However, these concepts are not too difficult if the fundamentals are understood in 1D and then extended to 3D.

Reciprocal Lattice and Reciprocal Crystals

Why study reciprocal lattices?

Often the concepts related to reciprocal lattice strikes terror in the minds of students. As we shall see this is not too difficult if concepts are first understood in 1D.

- A crystal resides in real space. The diffraction pattern[#] resides in Reciprocal Space.
- In a diffraction experiment *(powder diffraction using X-rays, selected area diffraction in a TEM)*, a part of this reciprocal space is usually sampled.
- The diffraction pattern from a crystal (in Fraunhofer diffraction geometry), consists of a periodic array of spots (sharp peaks of intensity).
- From the real lattice the reciprocal lattice can be *geometrically constructed*[☺]. The properties of the reciprocal lattice are 'inverse' of the real lattice → planes 'far away' in the real crystal are closer to the origin in the reciprocal lattice.
- As a real crystal can be thought of as decoration of a lattice with motif; a reciprocal crystal can be visualized as a Reciprocal Lattice decorated with a motif* of Intensities.
  - **Reciprocal Crystal = Reciprocal Lattice + Intensities as Motif***
- The reciprocal of the 'reciprocal lattice' is nothing but the real lattice!
- *Planes* in real lattice become *points* in reciprocal lattice and vice-versa.

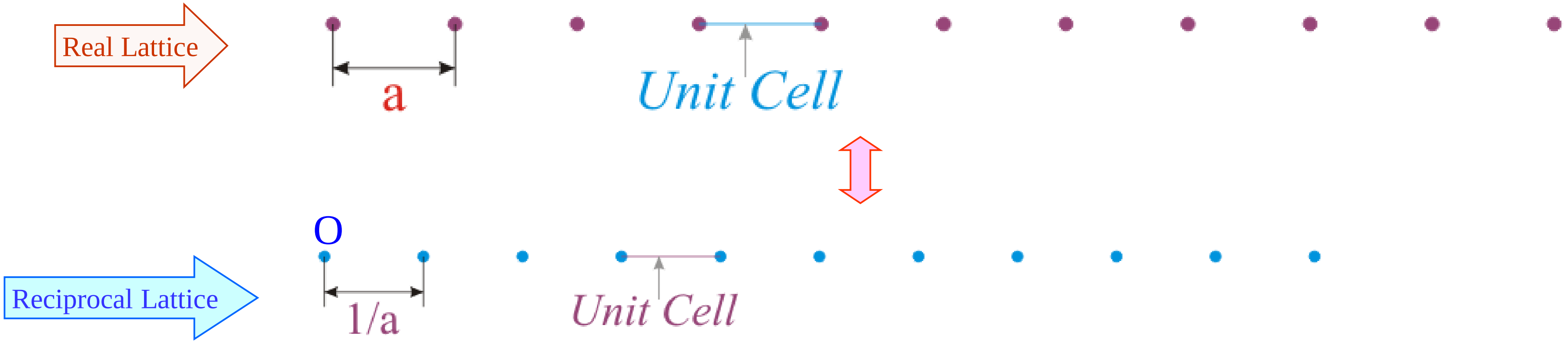
☺ *I.e. the information needed is the geometry of the lattice.*

* *Clearly, this is not the crystal motif- but a motif consisting of "Intensities".*

The complete diffraction pattern (not the one observed in an experiment)

We will construct reciprocal lattices in 1D and 2D before taking up a formal definition in 3D

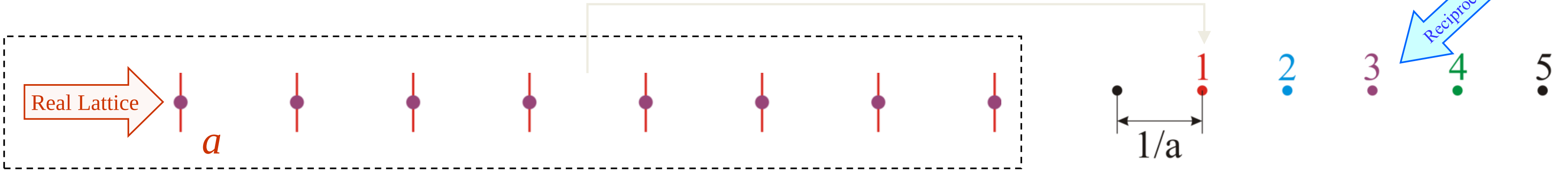
Let us start with a one dimensional lattice and construct the reciprocal lattice

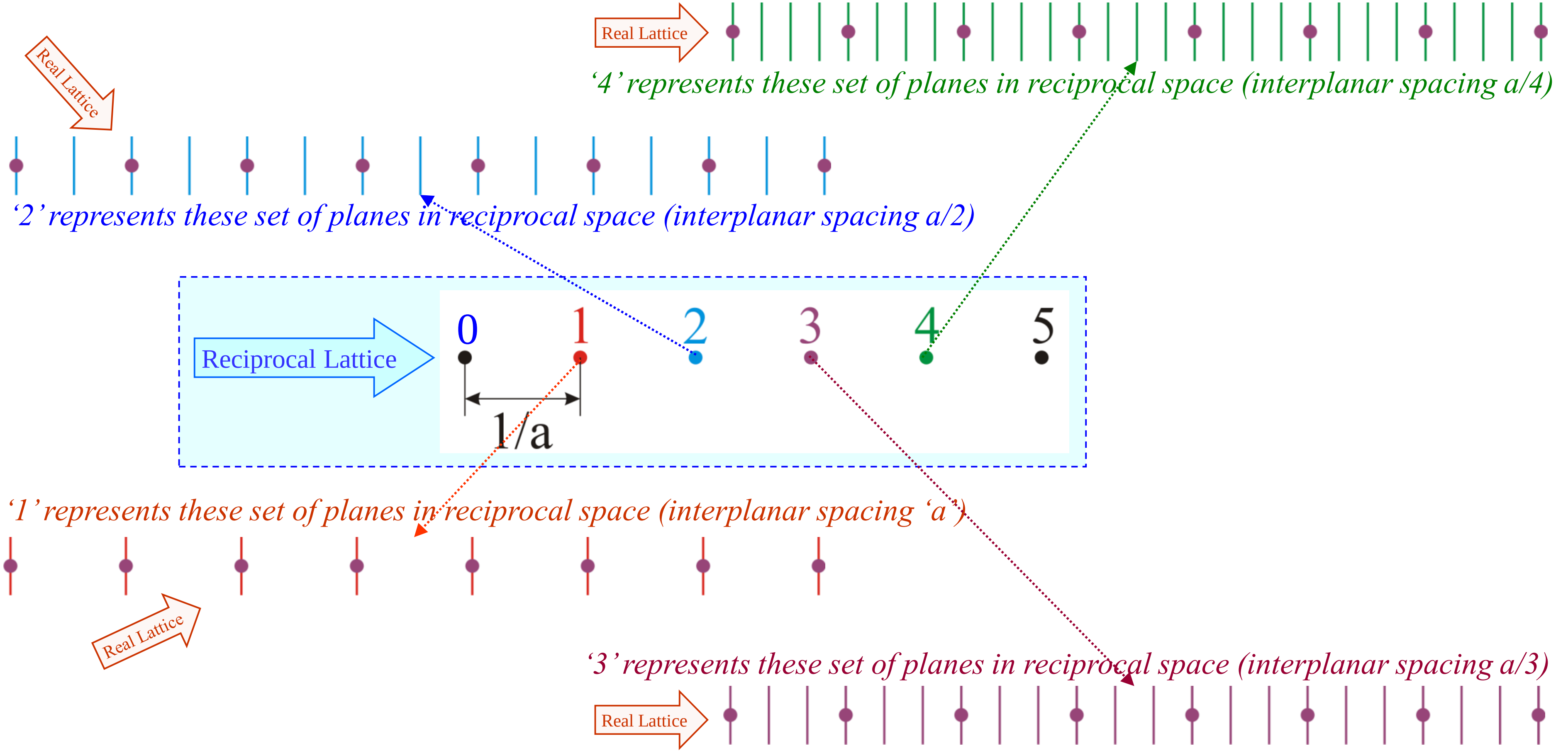


- The periodic array of points with lattice parameter ‘a’ is transformed to a reciprocal lattice with periodicity of ‘1/a’.
- The reciprocal lattice point at a distance of 1/a from the origin (O), represents the whole set of points (at a, 2a, 3a, 4a,….) in real space.
- The reciprocal lattice point at ‘2/a’ comes from a set of points with fractional lattice spacing a/2 (i.e. with periodicity of a/2). The lattice with periodicity of ‘a’ is a subset of this lattice with periodicity of a/2. *(Refer next slide)*.

Funda Check

What do the various points (with indices 1, 2, 3, 4… etc.) represent in real space?


'1' represents these set of planes in reciprocal space (interplanar spacing 'a')


'4' represents these set of planes in reciprocal space (interplanar spacing a/4)

'2' represents these set of planes in reciprocal space (interplanar spacing a/2)

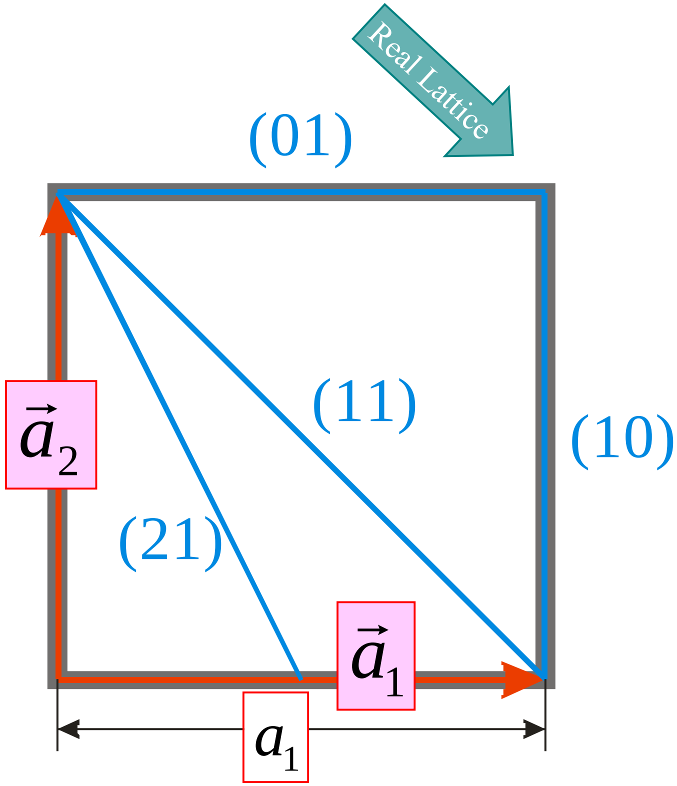
'1' represents these set of planes in reciprocal space (interplanar spacing 'a')

'3' represents these set of planes in reciprocal space (interplanar spacing a/3)

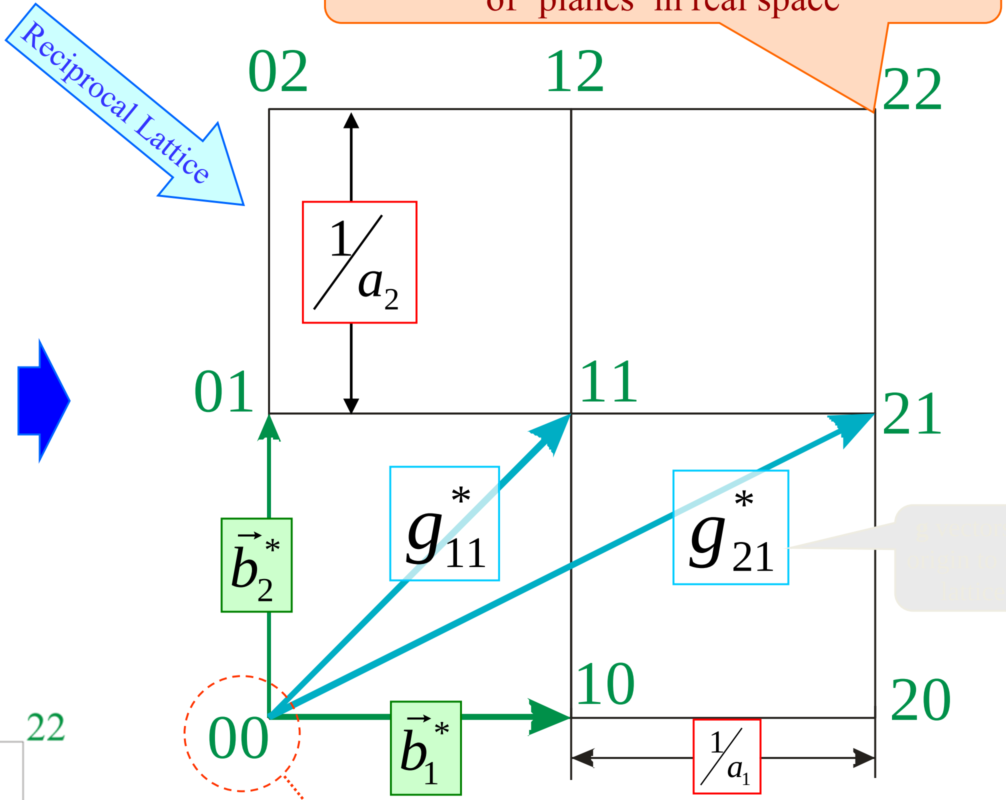
Note again: in 1D planes are points and have Miller indices of single digit (they have been extended into the second dimension (as lines) for better visibility and for the reason stated before).

Now let us construct some 2D reciprocal lattices

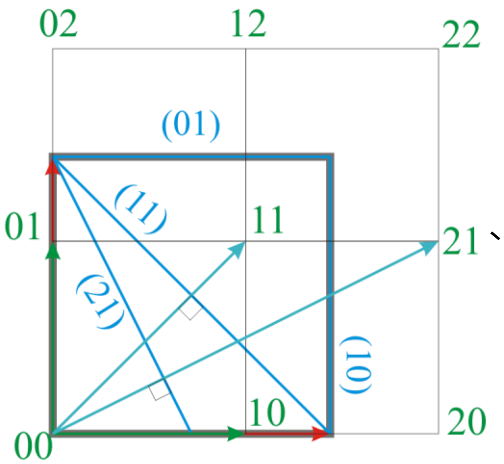
Example-1 Square lattice



Each one of these points correspond to a set of ‘planes’ in real space



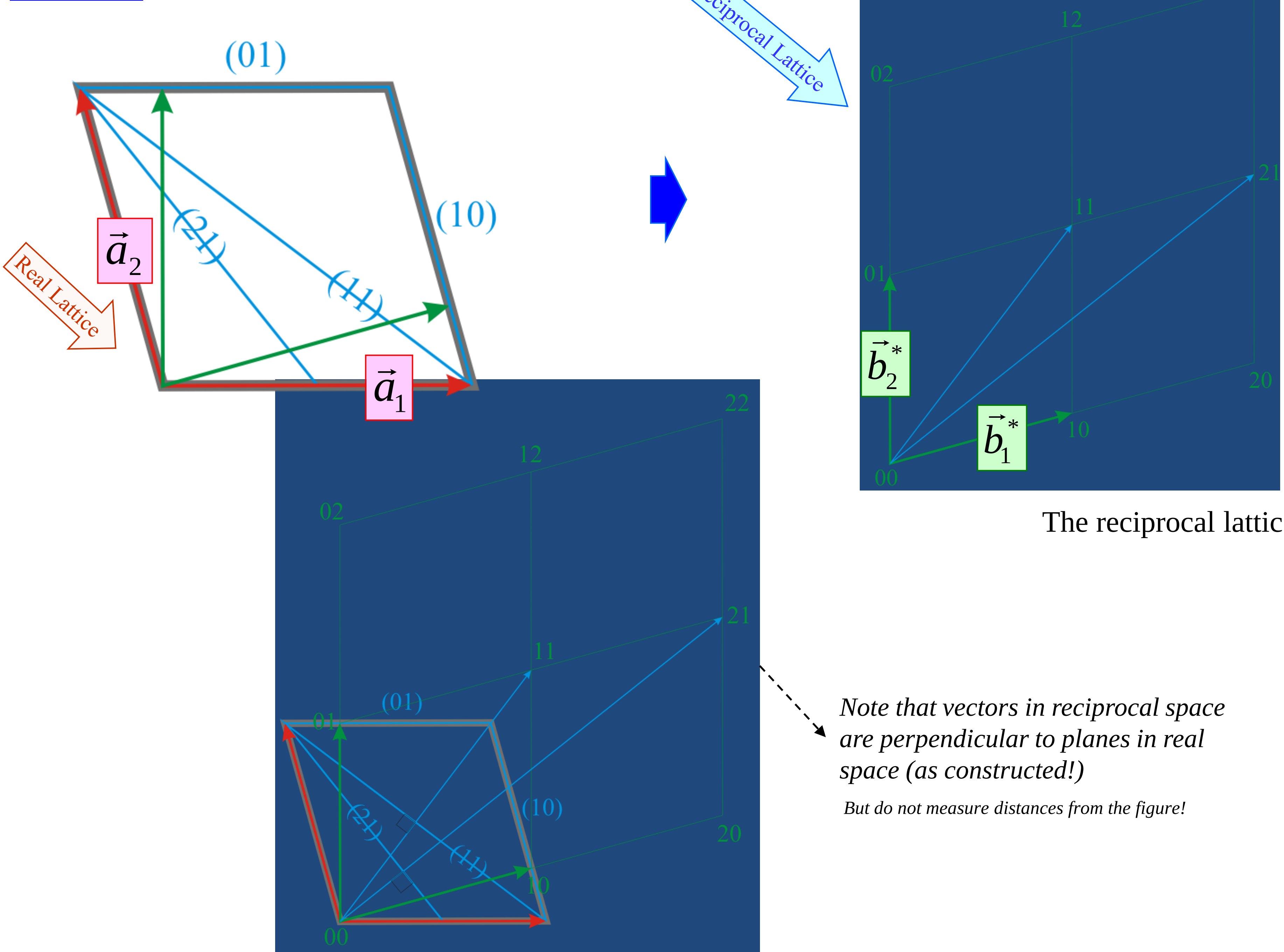
The reciprocal lattice has an origin!



Note that vectors in reciprocal space are perpendicular to planes in real space (as constructed!)

But do not measure distances from the figure!

Example-2 Oblique lattice (parallogram)



The reciprocal lattice

Note that vectors in reciprocal space are perpendicular to planes in real space (as constructed!)

But do not measure distances from the figure!

Reciprocal Lattice (3D)

Properties are reciprocal to the crystal lattice

- To get the reciprocal lattice in 3D, we need 3 basis vectors.
- These are defined using the basis vectors of the crystal as below, where V is the volume of the unit cell.
- The magnitude of the reciprocal lattice basis vector is (1/corresponding interplanar spacing).

BASIS VECTORS

$$\vec{b}_1^* = \frac{1}{V}(\vec{a}_2 \times \vec{a}_3)$$

$$\vec{b}_2^* = \frac{1}{V}(\vec{a}_3 \times \vec{a}_1)$$

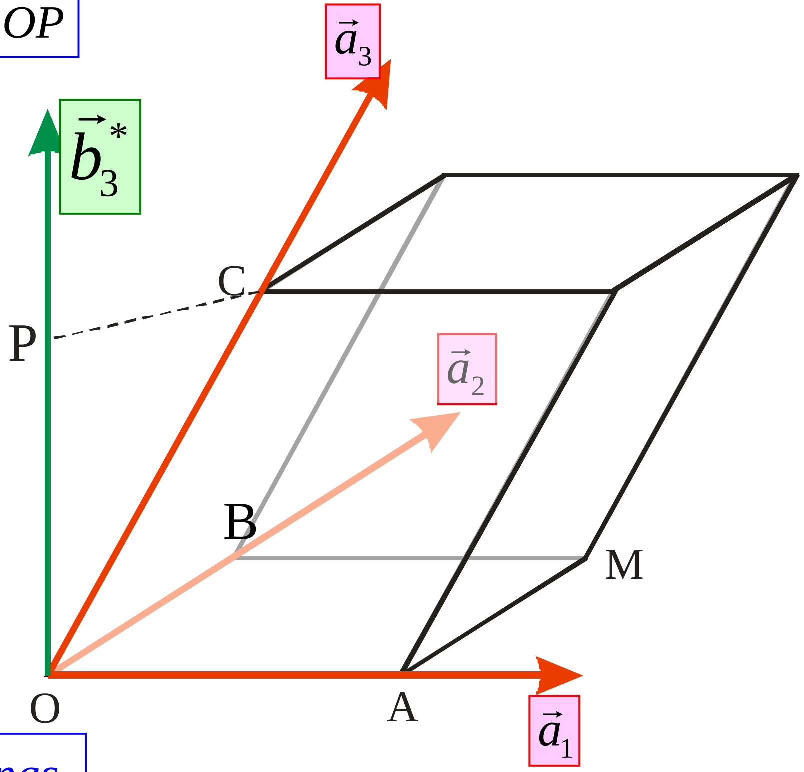
$$\vec{b}_3^* = \frac{1}{V}(\vec{a}_1 \times \vec{a}_2)$$

$\vec{b}_i^*$ is often written as $\vec{a}_i^*$

$$b_3^* = \left|\vec{b}_3^*\right| = \frac{1}{V}\left|(\vec{a}_1 \times \vec{a}_2)\right| = \frac{Area(OAMB)}{Area(OAMB)\cdot Height\ of\ Cell} = \frac{1}{OP}$$

$$b_3^* = \frac{1}{d_{001}}$$

$\vec{b}_3^*$ is $\perp$ to $\vec{a}_1$ *and* $\vec{a}_2$



The reciprocal lattice is created by interplanar spacings

Some properties of the reciprocal lattice and its relation to the real lattice

- A reciprocal lattice vector is ⊥ to the corresponding real lattice plane

$$\vec{g}^{\,*}_{hkl} = h\,\vec{b}_1^{\,*} + k\,\vec{b}_2^{\,*} + l\,\vec{b}_3^{\,*}$$

- The length of a reciprocal lattice vector is the reciprocal of the spacing of the corresponding real lattice plane

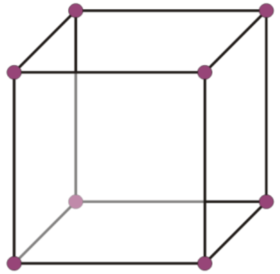
$$g^{*}_{hkl} = \left|\vec{g}^{\,*}_{hkl}\right| = \frac{1}{d_{hkl}}$$

- *Planes in the crystal become lattice points in the reciprocal lattice*
  - ➢ *Note that this is an alternate geometrical construction of the real lattice.*
- *Reciprocal lattice point represents the orientation and spacing of a set of planes.*

SC

Examples of 3D Reciprocal Lattices *weighed in with scattering power* ($|F|^2$)

Real Space

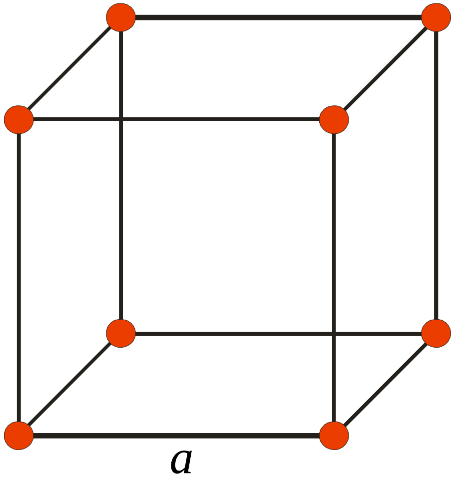


+

Single
sphere motif

Lattice = SC

=

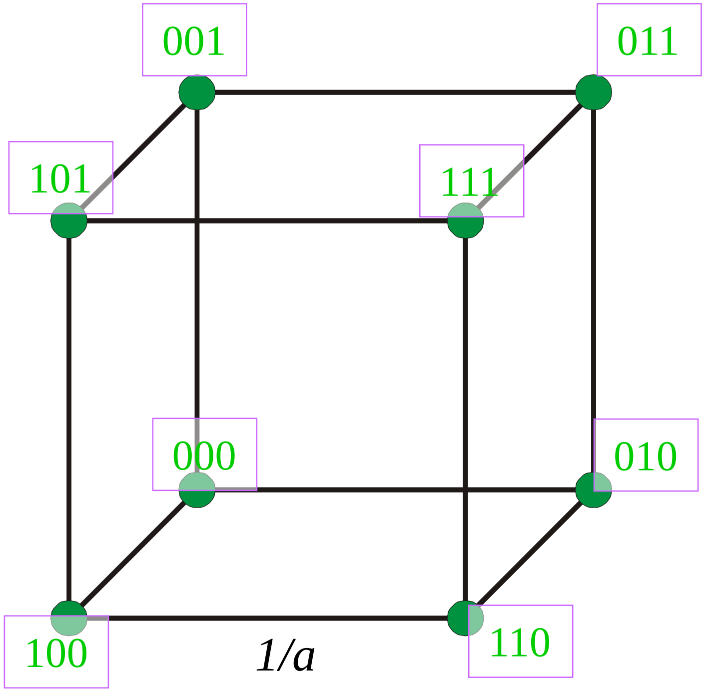


SC crystal

Reciprocal Space

Selection rule: All (hkl) allowed

In 'simple' cubic crystals there are No missing reflections

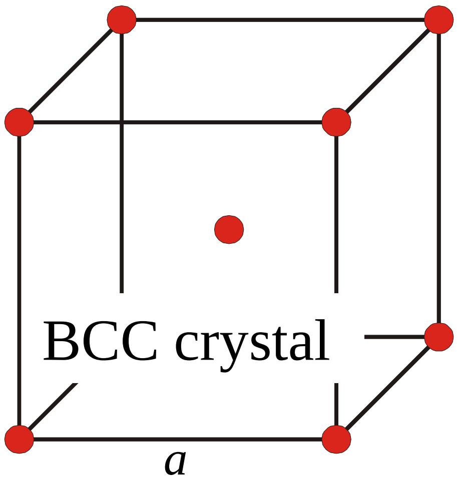


Reciprocal Crystal = SC

SC lattice with Intensities as the motif at each 'reciprocal' lattice point

Figures NOT to Scale

BCC

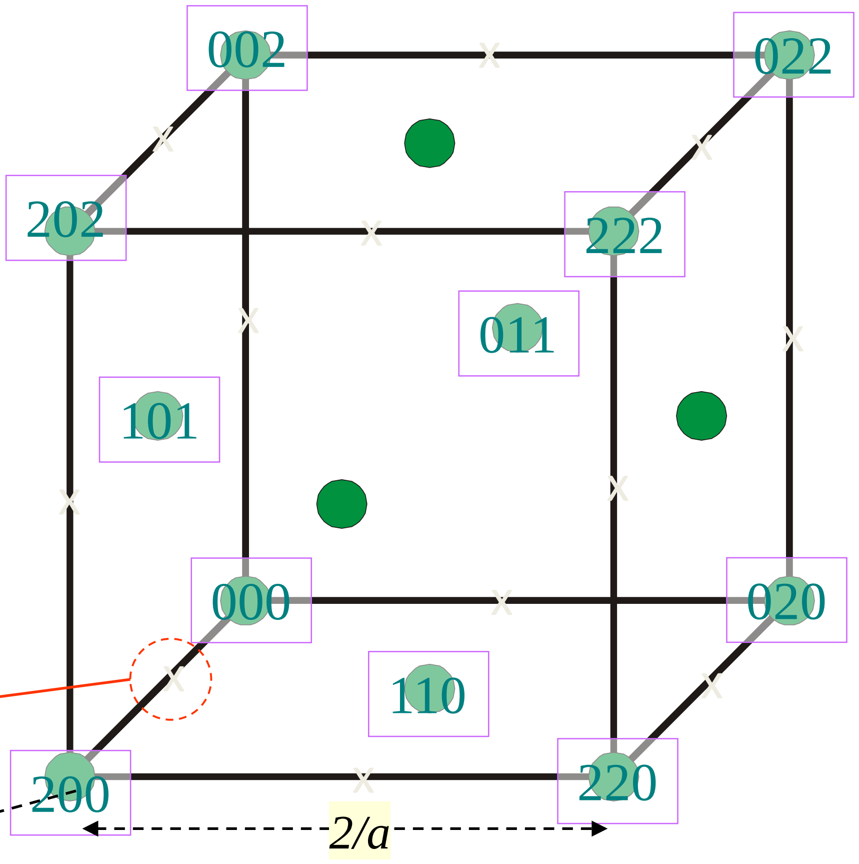


Selection rule BCC: (h+k+l) even allowed

In BCC 100, 111, 210, etc. go missing

Important note:

- The 100, 111, 210, etc. points in the reciprocal lattice exist (as the corresponding real lattice planes exist), however the intensity decorating these points is zero.



100 missing reflection (F = 0)

Weighing factor for each point "*motif*"

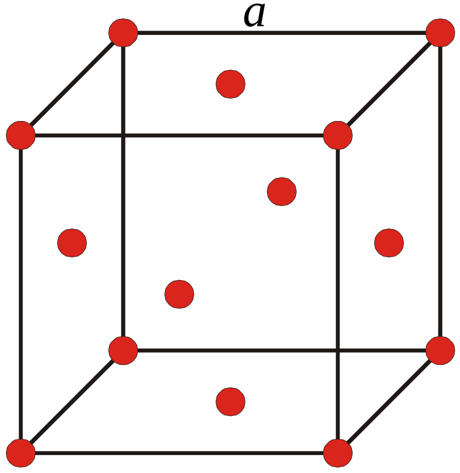
$$\boxed{F^2 = 4f^2}$$

Reciprocal Crystal = FCC

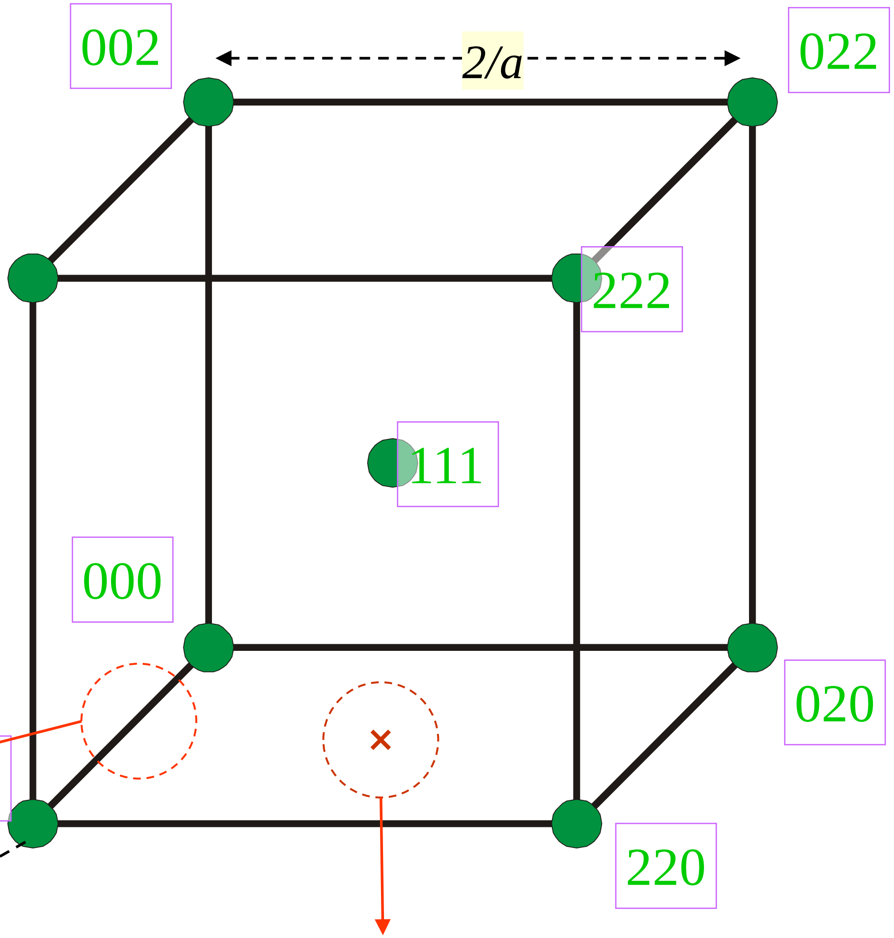
FCC lattice with Intensities as the motif

Figures NOT to Scale

FCC



Lattice = FCC



100 missing reflection (F = 0)

110 missing reflection (F = 0)

Weighing factor for each point “*motif*”

$$\boxed{F^2 = 16 f^2}$$

Reciprocal Crystal = BCC

BCC lattice with Intensities as the motif

Figures NOT to Scale